arXiv:0804.0067v1 [nucl-th] 1 Apr 2008

Global-Vector Representation of the Angular Motion of Few-Particle Systems II

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Abstract. The angular motion of a few-body system is described with global vectors which depend on the positions of the particles. The previous study using a single global vector is extended to make it possible to describe both natural and unnatural parity states. Numerical examples include three- and four-nucleon systems interacting via nucleon-nucleon potentials of AV8 type and a 3α system with a nonlocal $\alpha\alpha$ potential. The results using the explicitly correlated Gaussian basis with the global vectors are shown to be in good agreement with those of other methods. A unique role of the unnatural parity component, caused by the tensor force, is clarified in the 0_1^- state of ^{4}He. Two-particle correlation function is calculated in the coordinate and momentum spaces to show different characteristics of the interactions employed.

1 Introduction

Realistic nucleon-nucleon potentials contain strong tensor components. The tensor force induces the coupling of different orbital and spin angular momenta in the wave function of a few-nucleon system. Because of this property a variational solution of the system faces complexities in describing the orbital motion. There are two widely used methods to expand the orbital part of the wave function. One is a hyperspherical harmonics (HH) expansion [1, 2], and the other is a successive coupling of partial waves for the relative motion of the particles [3, 4, 5, 6, 7]. A converged solution is attained by increasing the orbital angular momenta.

Another representation for the orbital motion, proposed in refs. [8, 9], is to use a global vector (GV) which is defined by a linear combination of the relative coordinates. The coefficients of the combination determine the vector

responsible for the rotation of the system. The spherical part of the orbital motion is expressed in terms of an explicitly correlated Gaussian (CG). The efficiency of the GV representation (GVR) has been tested in many examples [10, 11, 12, 13] including not only nuclear but also atomic and hypernuclear physics problems. Its accuracy was confirmed in ref. [11] by comparing with the partial-wave expansion (PWE) for ^{3}H and α-particle interacting with central and tensor forces. In these studies only a single GV is used, and its application is thus restricted to natural parity states.

The purpose of this paper is to extend the GVR to describe the orbital motion with unnatural parity and to test the power of its representation. The unnatural parity state is usually unfavorable to gain the energies of low-lying levels, but it is needed to reach a precise energy particularly when the noncentral forces are taken into account. For example, the ground state of ^{4}He can be specified by three channels with (L, S)=(0,0), (1,1) and (2,2), where L and S are respectively the total orbital and spin angular momenta. Here the channel with L=1 and positive parity is unnatural, and its mixing probability is of order only $0.37\,\%$ [14]. However, the L=1 unnatural component gives rise to a contribution of more than $1\,\mathrm{MeV}$ to the ground state energy.

It is not a surprise that the interaction between composite particles like the nucleon becomes nonlocal [15], and indeed there is now available a new class of nonlocal nucleon-nucleon interactions, e.g., N^{3}LO [16] and low-k [17] potentials. The nonlocal operator also appears when one needs to eliminate some redundant or Pauli-forbidden states from the relative motion between composite particles [18]. Thus we take a certain class of nonlocal operators into consideration in the present paper.

A simple method of incorporating the unnatural parity state is to introduce two GVs. This was performed in the case of central forces and successfully applied to a search for excited states of a positronium molecule [19]. Here we develop a method of calculating the matrix elements of not only noncentral forces but also other local operators of physical interest such as a multipole density and some nonlocal operators.

The paper is organized as follows. The CG basis with two GVs is defined in Sect. 2 and its generating function is introduced. A nice property of the CG basis is that its Fourier transform is again the CG in momentum variables. A basic method of calculating matrix elements is explained in Sect. 3. The matrix element of a nonlocal operator between the generating functions is given in Sect. 4. In Sect. 5 we present results calculated for three- and four-nucleon systems using the two GVs and compare them to other calculations. As an example of the nonlocal potential, we consider a 3α system interacting via the nonlocal α-α potential derived from the resonating group method (RGM) [20]. A summary is drawn in Sect. 6. Formulas used in the present calculation are collected in Appendices. We give the CG basis in the momentum space in Appendix A, present the matrix elements of physically important operators in Appendix B, discuss the integral transform of the CG basis in Appendix C, and derive the matrix elements for some nonlocal operators in Appendix D.

2 Correlated Gaussian basis with double global vectors

The basis function in LS coupling scheme takes a form

$$\Phi_{(LS)JM_JTM_T} = [\psi_L^{(\text{space})}\psi_S^{(\text{spin})}]_{JM_J}\psi_{TM_T}^{(\text{isospin})}, \tag{2.1}$$

where the square bracket $[\dots]$ stands for the angular momentum coupling. The spin and isospin parts are expanded using the basis of successive coupling, e.g.,

$$\psi_{SM_S}^{(\text{spin})} = \big|[\cdots[[[\tfrac{1}{2}\tfrac{1}{2}]_{S_{12}}\tfrac{1}{2}]_{S_{123}}]\cdots]_{SM_S}\big\rangle. \tag{2.2}$$

Here the set of intermediate spins $(S_{12}, S_{123}, \dots)$ takes all possible values for a given S. The orbital part $\psi_{LM}^{(\text{space})}$ is expanded in terms of the CG basis which is explained in detail below. The symmetry of identical particles has to be imposed on the basis function.

2.1 Generating function for correlated Gaussian basis

Assuming that the system consists of N particles, we denote the single-particle coordinate of particle i by $\boldsymbol{r}_i$. It is convenient to introduce relative and center of mass coordinates, denoted $\boldsymbol{x}_i$, to describe intrinsic excitations of the system. Both coordinates are related to each other by a linear transformation

$$\boldsymbol{x}_i = \sum_{j=1}^{N} U_{ij}\boldsymbol{r}_j, \qquad \boldsymbol{r}_i = \sum_{j=1}^{N}(U^{-1})_{ij}\boldsymbol{x}_j, \tag{2.3}$$

where $\boldsymbol{x}_N$ is chosen to be the center of mass coordinate. Let $\boldsymbol{x}$ denote an $(N-1)$-dimensional column vector, excluding $\boldsymbol{x}_N$, whose ith element is a usual 3-dimensional vector $\boldsymbol{x}_i$. A choice of $\boldsymbol{x}$ often employed is the Jacobi set of coordinates, but may be any other set of relative coordinates.

A natural parity basis with the orbital angular momentum LM and parity $(-1)^L$ is described as

$$\exp\left(-\frac{1}{2}\widetilde{\boldsymbol{x}}A\boldsymbol{x}\right)\mathcal{Y}_{LM}(\widetilde{u_1}\boldsymbol{x}), \tag{2.4}$$

where $\mathcal{Y}_{LM}(\widetilde{u_1}\boldsymbol{x})$ is a solid spherical harmonics

$$\mathcal{Y}_{LM}(\widetilde{u_1}\boldsymbol{x}) = |\widetilde{u_1}\boldsymbol{x}|^L Y_{LM}(\widehat{\widetilde{u_1}\boldsymbol{x}}) \tag{2.5}$$

which is specified by a single GV, $\widetilde{u_1}\boldsymbol{x}=\sum_{i=1}^{N-1}u_{1_i}\boldsymbol{x}_i$. The symbol $\sim$ denotes the transpose of a matrix. In Eq. (2.4) A is an $(N-1)\times(N-1)$ positive-definite, symmetric matrix, and $\widetilde{\boldsymbol{x}}A\boldsymbol{x}$ is a short-hand notation for $\sum_{i,j=1}^{N-1}A_{ij}\boldsymbol{x}_i\cdot\boldsymbol{x}_j$. The matrix A and the $(N-1)$-dimensional column vector u_1 are parameters to characterize the "shape" of the basis function. The function (2.4) is a natural extension of $\exp(-\frac{1}{2}ar^2)\mathcal{Y}_{\ell m}(\boldsymbol{r})$ for a single variable case to many-particle system.

Another extension commonly used is a successive coupling of the partial waves corresponding to the respective coordinates, namely, $\exp(-\frac{1}{2}a_1\boldsymbol{x}_1^2-\frac{1}{2}a_2\boldsymbol{x}_2^2-\cdots)$ $[\cdots[[\mathcal{Y}_{\ell_1}(\boldsymbol{x}_1)\mathcal{Y}_{\ell_2}(\boldsymbol{x}_2)]_{L_{12}}\mathcal{Y}_{\ell_3}(\boldsymbol{x}_3)]_{L_{123}}\cdots]_{LM}$. The basis function (2.4) was

compared to that of PWE [11] and the GVR is found to be an excellent alternative to describe the rotational motion. The angular part was extended in refs. [10, 11] to $|\widetilde{u_1}\boldsymbol{x}|^{2K}\mathcal{Y}_{LM}(\widetilde{u_1}\boldsymbol{x})$, which was found to be advantageous to cope with short-ranged repulsive forces. We use the form (2.5) in this paper, however, since it greatly simplifies the calculation of matrix elements.

An unnatural parity basis with the angular momentum LM and parity $(-1)^{L+1}$ is described using two GVs as

$$\exp\left(-\frac{1}{2}\widetilde{\boldsymbol{x}}A\boldsymbol{x}\right)[\mathcal{Y}_L(\widetilde{u_1}\boldsymbol{x})\mathcal{Y}_1(\widetilde{u_2}\boldsymbol{x})]_{LM}, \qquad (2.6)$$

where u_2 is an $(N-1)$-dimensional column vector which defines the second GV. Both forms of Eqs. (2.4) and (2.6) are unified as

$$F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x}) = \exp\left(-\frac{1}{2}\widetilde{\boldsymbol{x}}A\boldsymbol{x}\right)[\mathcal{Y}_{L_1}(\widetilde{u_1}\boldsymbol{x})\mathcal{Y}_{L_2}(\widetilde{u_2}\boldsymbol{x})]_{LM}. \qquad (2.7)$$

That is, $L_1 = L$, $L_2 = 0$ for the natural parity case and $L_1 = L$, $L_2 = 1$ for the unnatural parity case. We stress that some important symmetry properties such as translation invariance and rotation invariance are already built in the basis (2.7). We show in Appendix A that the Fourier transform of Eq. (2.7) is again a combination of CG in momentum space.

The basis function introduced above provides us with a trial function for all states but $L = 0$ and a negative parity. The angular part of the basis for such a particular case must contain at least three vectors like $\boldsymbol{x}_i \cdot (\boldsymbol{x}_j \times \boldsymbol{x}_k)$ [19].

We present calculation formulas of matrix elements for the basis (2.7) with arbitrary L_1 and L_2 values for a given L. Formulas for some simple operators are already given in refs. [8, 9, 10, 12] for natural parity and in ref. [19] for unnatural parity. In the appendices we give formulas for various operators including noncentral potentials as well as those nonlocal kernels which appear in the RGM formulation for nuclear cluster models [20].

Our method is based on the use of the generating function g for the CG:

$$g(\boldsymbol{s}; A, \boldsymbol{x}) = \exp\left(-\frac{1}{2}\widetilde{\boldsymbol{x}}A\boldsymbol{x} + \widetilde{\boldsymbol{s}}\boldsymbol{x}\right), \qquad (2.8)$$

where $\boldsymbol{s}$ is an $(N-1)$-dimensional column vector whose ith element is a 3-dimensional vector $\boldsymbol{s}_i$. By expressing $\boldsymbol{s}_i$ with 3-dimensional unit vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ as $\boldsymbol{s}_i = \lambda_1\boldsymbol{e}_1u_{1_i}+\lambda_2\boldsymbol{e}_2u_{2_i}$, the basis function (2.7) is generated as follows:

$$F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x}) = \frac{B_{L_1}B_{L_2}}{L_1!L_2!}\int\int d\boldsymbol{e}_1\,d\boldsymbol{e}_2\,[Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)]_{LM}$$

$$\times\frac{\partial^{L_1+L_2}}{\partial\lambda_1^{L_1}\partial\lambda_2^{L_2}}\,g(\lambda_1\boldsymbol{e}_1u_1+\lambda_2\boldsymbol{e}_2u_2; A, \boldsymbol{x})\Big|_{\lambda_1=\lambda_2=0}, \quad (2.9)$$

where

$$B_L = \frac{(2L+1)!!}{4\pi}. \qquad (2.10)$$

When $g(\lambda_1\boldsymbol{e}_1u_1 + \lambda_2\boldsymbol{e}_2u_2; A, \boldsymbol{x})$ is expanded in powers of λ_1, only the term of degree $\lambda_1^{L_1}$ contributes in Eq. (2.9), and this term contains the L_1-th degree

of $\boldsymbol{e}_1$ because λ_1 and $\boldsymbol{e}_1$ always appear simultaneously. In order for the term to contribute to the integration over $\boldsymbol{e}_1$, these L_1 vectors of $\boldsymbol{e}_1$ must couple to the angular momentum L_1, that is they are uniquely coupled to the maximum possible angular momentum. The same applies to λ_2 as well.

2.2 Coordinate transformation

Suppose that the coordinate set $\boldsymbol{x}$ is transformed to a new set of relative coordinates $\boldsymbol{y}$ through $\boldsymbol{y} = \mathcal{P}\boldsymbol{x}$ with an $(N-1) \times (N-1)$ matrix $\mathcal{P}$. The transformation of this kind is needed, e.g., when the permutation symmetry of the constituent particles is imposed on the basis function or different coordinate sets are used to describe particular correlated motion [4]. The CG basis function in the coordinate set $\boldsymbol{y}$ is rewritten as

$$F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{y}) = F_{(L_1L_2)LM}(u_{\mathcal{P}1}, u_{\mathcal{P}2}, A_{\mathcal{P}}, \boldsymbol{x}) \tag{2.11}$$

with

$$A_{\mathcal{P}} = \widetilde{\mathcal{P}}A\mathcal{P}, \qquad u_{\mathcal{P}1} = \widetilde{\mathcal{P}}u_1, \qquad u_{\mathcal{P}2} = \widetilde{\mathcal{P}}u_2. \tag{2.12}$$

The coordinate transformation ends up redefining A, u_1 and u_2 as above, and we do not need to introduce different coordinate sets. This property that the functional form of the CG remains unchanged under the coordinate transformation enables one to unify the method of calculating the matrix element.

3 Calculation of matrix elements

We introduce the following abbreviated notation for a matrix element

$$\langle F'|\mathcal{O}|F\rangle \equiv \langle F_{(L_3L_4)L'M'}(u_3, u_4, A', \boldsymbol{x})|\mathcal{O}|F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle, \tag{3.1}$$

where $\mathcal{O}$ stands for an operator of interest. Using Eq. (2.9) in Eq. (3.1) enables one to relate the matrix element to that between the generating functions:

$$\begin{aligned}
\langle F'|\mathcal{O}|F\rangle &= \left(\prod_{i=1}^{4} \frac{B_{L_i}}{L_i!} \int d\boldsymbol{e}_i\right) ([Y_{L_3}(\boldsymbol{e}_3)Y_{L_4}(\boldsymbol{e}_4)]_{L'M'})^* [Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)]_{LM} \\
&\quad \times \left(\prod_{i=1}^{4} \frac{\partial^{L_i}}{\partial \lambda_i^{L_i}}\right) \langle g(\boldsymbol{s}'; A', \boldsymbol{x})|\mathcal{O}|g(\boldsymbol{s}; A, \boldsymbol{x})\rangle \Big|_{\lambda_1=\lambda_2=\lambda_3=\lambda_4=0}
\end{aligned} \tag{3.2}$$

with

$$\boldsymbol{s} = \lambda_1\boldsymbol{e}_1 u_1 + \lambda_2\boldsymbol{e}_2 u_2, \qquad \boldsymbol{s}' = \lambda_3\boldsymbol{e}_3 u_3 + \lambda_4\boldsymbol{e}_4 u_4. \tag{3.3}$$

The calculation of the matrix element consists of three stages:

1. Calculate the matrix element,

    $$\mathcal{M} = \langle g(\lambda_3\boldsymbol{e}_3 u_3 + \lambda_4\boldsymbol{e}_4 u_4; A', \boldsymbol{x})|\mathcal{O}|g(\lambda_1\boldsymbol{e}_1 u_1 + \lambda_2\boldsymbol{e}_2 u_2; A, \boldsymbol{x})\rangle,$$

    between the generating functions.

2. Expand $\mathcal{M}$ in powers of λ_i and keep only those terms of degree L_i for each i. The terms should contain the unit vector $\boldsymbol{e}_i$ of degree L_i as well. One may drop any term with $\lambda_i^2\boldsymbol{e}_i \cdot \boldsymbol{e}_i = \lambda_i^2$ etc.

3. Perform the differentiation and integration prescribed in Eq. (3.2).

Formulas for most important matrix elements $\mathcal{M}$ are tabulated in ref. [9]. The angle integration in stage 3 can be performed using a formula

$$\int \cdots \int \prod_{i=1}^{4} d\boldsymbol{e}_i ([Y_{L_3}(\boldsymbol{e}_3)Y_{L_4}(\boldsymbol{e}_4)]_{L'M'})^*[Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)]_{LM}$$

$$\times [[Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)]_L[Y_{L_3}(\boldsymbol{e}_3)Y_{L_4}(\boldsymbol{e}_4)]_{L'}]_{\kappa\mu}$$

$$= (-1)^{L-L'+\kappa+L_1+L_2}\sqrt{\frac{2\kappa+1}{2L'+1}}\langle LM\kappa\mu|L'M'\rangle. \tag{3.4}$$

Appendix B collects formulas for the matrix elements of some local operators.

4 Basic matrix elements for nonlocal operators

Let us consider the matrix element of a nonlocal operator acting between particles k and l. The relative distance vector, $\boldsymbol{r}_k-\boldsymbol{r}_l$, can be expressed as a linear combination of $\boldsymbol{x}_i$ (excluding the center of mass coordinate $\boldsymbol{x}_N$) as

$$\boldsymbol{r}_k - \boldsymbol{r}_l = \sum_{i=1}^{N-1} w_i\boldsymbol{x}_i = \widetilde{w}\boldsymbol{x}, \tag{4.1}$$

where the $(N-1)$-dimensional column vector w is given by

$$w_i = (U^{-1})_{ki} - (U^{-1})_{li}. \tag{4.2}$$

See Eq. (2.3). The nonlocal operator may in general be expressed as

$$V_{\text{NL}} = \int\int d\boldsymbol{r}\, d\boldsymbol{r}'\, V(\boldsymbol{r}',\boldsymbol{r})\, |\delta(\widetilde{w}\boldsymbol{x}-\boldsymbol{r}')\rangle\langle\delta(\widetilde{w}\boldsymbol{x}-\boldsymbol{r})|, \tag{4.3}$$

where $V(\boldsymbol{r}',\boldsymbol{r})$ determines the form factor of the nonlocal operator.

The operator of type (4.3) was applied to the study of α-cluster condensation in ^{12}C and ^{16}O [21]. Evaluating the matrix element of the nonlocal operator requires deliberation because the coordinate $\widetilde{w}\boldsymbol{x}$ has to be singled out from the set of $(N-1)$ coordinates $\boldsymbol{x}_i$, and because the rest of other $(N-2)$ coordinates must be properly defined on the condition that they are all independent of $\widetilde{w}\boldsymbol{x}$. Though the choice of these $(N-2)$ coordinates is not unique, the matrix element should not depend on its choice. This problem is discussed in Appendix C.

As derived in Appendix D.1, the basic matrix element reads

$$\langle g(\boldsymbol{s}';A',\boldsymbol{x}) \mid V_{\text{NL}} \mid g(\boldsymbol{s};A,\boldsymbol{x})\rangle = \left(\frac{(2\pi)^{N-2}c}{\det B}\right)^{\frac{3}{2}}\exp\left(\frac{1}{2}(\widetilde{\boldsymbol{s}}+\widetilde{\boldsymbol{s}}')J^{-1}(\boldsymbol{s}+\boldsymbol{s}')\right)$$

$$\times \int\int d\boldsymbol{r}' d\boldsymbol{r} V(\boldsymbol{r}',\boldsymbol{r})\exp\left(-\frac{1}{2}\alpha'\boldsymbol{r}'^2 - \frac{1}{2}\alpha\boldsymbol{r}^2 - \beta\boldsymbol{r}'\cdot\boldsymbol{r}\right)$$

$$\times \exp\left([(\widetilde{\zeta}-\widetilde{\eta}')\boldsymbol{s}' - \widetilde{\eta}'\boldsymbol{s}]\cdot\boldsymbol{r}' + [(\widetilde{\zeta}-\widetilde{\eta})\boldsymbol{s} - \widetilde{\eta}\boldsymbol{s}']\cdot\boldsymbol{r}\right), \tag{4.4}$$

where

$$B = A + A', \qquad c = (\widetilde{w}B^{-1}w)^{-1}, \qquad J^{-1} = B^{-1} - cB^{-1}w\widetilde{w}B^{-1}, \qquad (4.5)$$

and

$$a = \widetilde{\zeta}A\zeta, \qquad a' = \widetilde{\zeta}A'\zeta, \qquad \eta = J^{-1}A\zeta, \qquad \eta' = J^{-1}A'\zeta,$$

$$\alpha = a - \widetilde{\zeta}A\eta, \qquad \alpha' = a' - \widetilde{\zeta}A'\eta', \qquad \beta = -\frac{1}{2}\widetilde{\zeta}(A\eta' + A'\eta). \qquad (4.6)$$

Here ζ is an $(N-1)$-dimensional column vector that is determined uniquely from w defined in Eq. (4.1). See Appendix C.2.

We perform the integration in Eq. (4.4) for a given $V(\boldsymbol{r}',\boldsymbol{r})$ and follow the procedure described in Sect. 3. Some examples are collected in Appendix D.

5 Numerical results

5.1 Spectroscopic properties of few-nucleon systems

A few-nucleon system interacting via a realistic two-body force offers good examples of testing the CG basis function with the GVR. The N-nucleon system is specified by the following Hamiltonian

$$H = \sum_{i=1}^{N} T_i - T_{\text{cm}} + \sum_{j>i=1}^{N} v_{ij}. \qquad (5.1)$$

Three-body forces are neglected though their inclusion does not cause any problem. The operator T_i is a kinetic energy and the center of mass kinetic energy T_{cm} is subtracted in the Hamiltonian. A realistic nucleon-nucleon force is characterized by a short-ranged repulsion and a long-ranged tensor force. To clarify the role of these properties, we employ three types of potential models as v_{ij}. The first is the Minnesota (MN) potential [22] which contains rather mild short-ranged repulsion and renormalizes the effect of the tensor force into its central term. No spin-orbit component of the MN potential is included. The second is the AV8$'$ potential [23] which is obtained from the Argonne V18 potential with a suitable renormalization procedure. The AV8$'$ potential consists of central, tensor and spin-orbit terms. A few-body calculation with this potential shows slow convergence because of its strong short-ranged repulsion, and in addition the radial form factor of AV8$'$ makes the evaluation of matrix elements time-consuming in the present approach. The third is the G3RS potential [24] whose radial form is given as a combination of Gaussians with three ranges, which makes the numerical calculation much faster. Other features of the G3RS potential compared to AV8$'$ are that the central force is deep, the tensor force is weak and the repulsion at the origin is mild. The original G3RS potential contains $\boldsymbol{L}^2$ and quadratic $\boldsymbol{L}\cdot\boldsymbol{S}$ terms in even partial waves. The contribution of these terms is small [25], and they are ignored in the present calculation.

The form of v is written as

$$v_{12} = V_{\text{c}}(r) + V_{\text{Coul}}(r)P_{1\pi}P_{2\pi} + V_{\text{t}}(r)S_{12} + V_{\text{b}}(r)\boldsymbol{L}\cdot\boldsymbol{S}, \qquad (5.2)$$

where S_{12} and $\boldsymbol{L}\cdot\boldsymbol{S}$ stand for the tensor and spin-orbit operators and $P_{i\pi}=1$ for proton and 0 for neutron. The neutron projection operator $P_{i\nu}$ is defined in a similar way. The inputs used in this subsection are $\hbar^2/m_N=41.47106$ MeV fm^2 and $e^2=1.440$ MeV fm. Here m_N is the nucleon mass, and the mass difference between proton and neutron is ignored. No isospin mixture is taken into account. The u parameter of the MN potential is set to $u=1$.

The wave function of the system is expressed as a combination of different channel components specified with L and S (see Eq. (2.1)):

$$\Psi = \sum_{LS} X_{LS}\Psi_{(LS)JM_JTM_T}, \tag{5.3}$$

where $\Psi_{(LS)JM_JTM_T}$ is assumed to be normalized. The squared coefficient

$$P(L,S) = (X_{LS})^2 \tag{5.4}$$

denotes the probability of finding the system in the channel (L,S). Possible channels for the ground states of $N \leq 4$ systems are $(L,S)=(0,1)$, $(2,1)$ for deuteron, $(0,1/2)$, $(2,3/2)$, $(1,1/2)$, $(1,3/2)$ for ^{3}H and ^{3}He, and $(0,0)$, $(2,2)$, $(1,1)$ for α-particle. Among these channels, $(1,1/2)$ and $(1,3/2)$ for ^{3}H (^{3}He) and $(1,1)$ for α-particle are unnatural parity. Table 1 compares the deuteron properties calculated with the three potentials. Comparing the result between AV8$'$ and G3RS, we see that the AV8$'$ potential is stronger in the tensor and spin-orbit components but weaker in the central component than the G3RS potential, as already noted above.

The orbital part of the full wave function is expanded in terms of the CG (2.7). The CG for the natural parity state has $L_1=L$ and $L_2=0$, and contains the parameters A and u_1, while the one for the unnatural parity state has $L_1=L$ and $L_2=1$, and contains A, u_1 and u_2. These parameters are selected by the stochastic variational method (SVM) [8, 9] as follows: First, we randomly choose a channel specified by L_i, L, S from among those (L,S) channels which are included in the calculation. For a given S value, a set of intermediate spins is randomly chosen. For example, for three-nucleon system with $S=1/2$, $|[[\frac{1}{2}\frac{1}{2}]_0\frac{1}{2}]_{1/2\,M_S}\rangle$ or

Table 1. Comparison of deuteron properties calculated with the different potentials. The energy and point nucleon root mean square (rms) radius are given in MeV and fm, respectively. The probability $P(L, S)$ is given in %.

Potential	MN	G3RS	AV8$'$
E	-2.202	-2.277	-2.242
$\langle T \rangle$	10.487	16.478	19.881
$\langle V_c \rangle$	-12.689	-7.294	-4.458
$\langle V_t \rangle$	–	-11.460	-16.641
$\langle V_b \rangle$	–	–	-1.024
$\sqrt{\langle r^2 \rangle}$	1.952	1.979	1.961
$P(0,1)$	100	95.22	94.23
$P(2,1)$	–	4.78	5.77

$|[[\frac{1}{2}\frac{1}{2}]_1\frac{1}{2}]_{1/2\,M_S}\rangle$ is randomly chosen. A set of intermediate isospins is chosen randomly as well. After choosing these discrete sets, we determine the nonlinear parameters A, u_i following the SVM procedure. The elements of A are chosen randomly from a physically important interval. The diagonal and off-diagonal elements of A describe the correlated motion of the system. The parameter u_i is also chosen randomly under the condition $\widetilde{u}_i u_i=1$. This parameter serves to express the partial waves needed to represent the rotational motion but its role is usually not as important as that played by A. Therefore we make more efforts to select a suitable A.

We decrease the energy first by increasing the number of basis functions one by one up to a certain dimension. Keeping the number of basis functions fixed, we then switch to a refinement process [8, 9] in which each basis function already selected is tested against other randomly chosen candidates. We repeat these two optimization procedures until a fair convergence is attained. When the number of basis functions becomes large enough to get a converged solution, it is convenient to rearrange the selected basis set according to importance. By the importance we mean the following. Suppose that the number of the basis functions is K. The first basis Φ_1 is the one that gives the lowest energy among the K functions. The second basis Φ_2 is the one that gives the lowest energy together with Φ_1 among the $K-1$ functions excluding Φ_1. This ordering is continued until the last basis Φ_K is determined. After rearranging the basis functions in this way, we often have those Φ_i which play a very minor role in lowering energy. This is the case particularly when i is close to K. These inactive bases may be discarded from the basis set to save the basis dimension. After this contraction of the basis set, we may again enlarge the basis dimension to search for better basis functions.

Table 2 lists the energies of three- and four-nucleon systems and the contributions of the respective terms of the Hamiltonian together with the nucleon rms radii. The GVR performance is tested by comparing to other calculations, particularly PWE calculations. The basis function in PWE is also Gaussian but no explicit correlated terms between the different coordinates are included, so that the matrix A is always chosen to be diagonal. A correlated motion is, however, accounted for by expanding the trial wave function in different coordinate sets. For example, both coordinates of K- and H-types are employed to obtain the solution for α-particle. Thus this PWE calculation is the same as the SVM of ref. [14], and its accuracy is well tested. A noteworthy difference between GVR and PWE is that the latter expresses the angular part of the wave function by successively coupling the partial waves ℓ_i to the resultant L. In the present calculation ℓ_i is restricted to $\ell_i \leq 2$. The total energy of ^{3}H calculated with AV8′ and its decomposition to each term agrees with the results of PWE and Faddeev [26]. The agreement between the GVR and PWE calculations is also very good for the properties of the α-particle. The four-nucleon system is solved by the different methods [14] using the AV8′ potential with the Coulomb force being neglected. If the Coulomb contribution of the present calculation is omitted, the GVR energy becomes $-25.85\,\mathrm{MeV}$, which agrees with the lowest energy of the benchmark calculations within $70\,\mathrm{keV}$. These results confirm that the CG basis with GVR is versatile enough to provide us with such accurate solutions that

Table 2. The ground state properties of three- and four-nucleon systems. The energy and rms radius are given in MeV and fm. The probability $P(L, S)$ is given in %. The basis dimensions for ^{4}He are 400 (G3RS) and 600 (AV8$'$) in GVR, and reduced to half in PWE, respectively.

Potential	MN	G3RS		AV8$'$		
Method	GVR	GVR	PWE	GVR	PWE	Ref. [26]
^{3}H($\frac{1}{2}^+$)						
E	-8.38	-7.73	-7.72	-7.76	-7.76	-7.767
$\langle T \rangle$	27.21	40.24	40.22	47.59	47.57	47.615
$\langle V_{\rm c} \rangle$	-35.59	-26.80	-26.79	-22.50	-22.49	-22.512
$\langle V_{\rm t} \rangle$	$-$	-21.13	-21.13	-30.85	-30.84	-30.867
$\langle V_{\rm b} \rangle$	$-$	-0.03	-0.03	-2.00	-2.00	-2.003
$\sqrt{\langle r^2 \rangle}$	1.71	1.79	1.79	1.75	1.75	
$P(0, 1/2)$	100	92.95	92.94	91.38	91.37	91.35
$P(2, 3/2)$	$-$	7.01	7.02	8.55	8.57	8.58
$P(1, 1/2)$	$-$	0.03	0.03	0.04	0.04	$\}0.07$
$P(1, 3/2)$	$-$	0.02	0.02	0.02	0.02	
^{3}He($\frac{1}{2}^+$)						
E	-7.71	-7.08	-7.08	-7.10	-7.10	
$\langle T \rangle$	26.69	39.46	39.43	46.68	46.67	
$\langle V_{\rm c} \rangle$	-35.06	-26.26	-26.24	-22.00	-21.98	
$\langle V_{\rm Coul} \rangle$	0.67	0.64	0.64	0.65	0.65	
$\langle V_{\rm t} \rangle$	$-$	-20.89	-20.88	-30.47	-30.47	
$\langle V_{\rm b} \rangle$	$-$	-0.03	-0.03	-1.97	-1.97	
$\sqrt{\langle r^2 \rangle}$	1.74	1.82	1.82	1.79	1.79	
$P(0, 1/2)$	100	92.98	92.96	91.42	91.41	
$P(2, 3/2)$	$-$	6.98	6.99	8.51	8.53	
$P(1, 1/2)$	$-$	0.03	0.03	0.04	0.04	
$P(1, 3/2)$	$-$	0.02	0.02	0.02	0.02	
^{4}He(0^+)						
E	-29.94	-25.29	-25.26	-25.08	-25.05	
$\langle T \rangle$	58.08	86.93	86.77	101.59	101.36	
$\langle V_{\rm c} \rangle$	-88.86	-66.24	-66.11	-54.93	-54.73	
$\langle V_{\rm Coul} \rangle$	0.83	0.76	0.76	0.77	0.77	
$\langle V_{\rm t} \rangle$	$-$	-46.62	-46.55	-67.85	-67.79	
$\langle V_{\rm b} \rangle$	$-$	-0.13	-0.12	-4.65	-4.66	
$\sqrt{\langle r^2 \rangle}$	1.41	1.51	1.51	1.49	1.49	
$P(0, 0)$	100	88.46	88.50	85.76	85.79	
$P(2, 2)$	$-$	11.30	11.26	13.87	13.85	
$P(1, 1)$	$-$	0.25	0.24	0.36	0.36	

are comparable to state-of-the-art calculations available in literatures.

We note from the comparison between AV8$'$ and G3RS results that the solution with AV8$'$ has large kinetic energy corresponding to the strong short-ranged repulsion. The tensor contribution is larger than the central force contribution in

AV8$'$. On the contrary, the G3RS potential gives larger attraction in the central contribution than in the tensor contribution. Though they give different potential contributions, both lead to almost the same total energy and nucleon rms radius. These features of the realistic potentials are very consistent with those of Table 1 listed for the deuteron.

Now we discuss how well the GVR can incorporate unnatural parity components. The unnatural parity state is usually unfavored because it has a larger kinetic energy than the natural parity state and its diagonal matrix element becomes rather high. If the off-diagonal matrix elements between the unnatural parity and natural parity states are large enough to compensate the loss of the kinetic energy, the mixing of the unnatural parity state becomes important. Table 3 lists the decomposition of the energies of ^{3}H and α-particle according to the (L, S) channel. The value for the diagonal channel denotes $(X_{LS})^2 \langle \Psi_{(LS)JM_JTM_T} | H | \Psi_{(LS)JM_JTM_T} \rangle$, while the value between the different channels is $2X_{LS}X_{L'S'} \langle \Psi_{(LS)JM_JTM_T} | H | \Psi_{(L'S')JM_JTM_T} \rangle$. Note that, in the case of ^{3}H, the contributions from the two spin channels of S=1/2 and 3/2 with the unnatural parity of L=1 are summed together. The probability of the unnatural parity state is negligibly small in ^{3}H, as shown in Table 2. The probability of the unnatural parity state $P(1,1)$ for α-particle increases to 0.25 % for G3RS and 0.36 % for AV8$'$. With this mixing of the unnatural parity component the tensor coupling with the (22) channel becomes important and thus the α-particle gains energy by about 0.8 MeV for G3RS and 1.6 MeV for AV8$'$.

The 0_1^- excited state of ^{4}He, located at 7.19 MeV below the $p+p+n+n$ threshold, is a very good example to demonstrate the importance of the unnatural parity state. The 0_1^- state consists of two channels, (L, S)=(1, 1) (natural parity) and (2, 2) (unnatural parity). The matrix element of each operator in the Hamiltonian is listed in Table 4 for the 0_1^- state, with the column-row index of the matrix being labeled by the channel, $(1, 1)$ or $(2, 2)$. The values in parentheses stand for the matrix elements, $\langle \Psi_{(LS)JM_JTM_T} | H | \Psi_{(L'S')JM_JTM_T} \rangle$ etc. The table confirms that the 0_1^- state cannot be predicted well below the $p+p+n+n$ threshold if the coupling of the two channels is neglected. The diagonal ma-

Table 3. Total energies, in MeV, of ^{3}H and α-particle decomposed into different (L, S) contributions.

^{3}H($\frac{1}{2}^+$)	G3RS			AV8$'$		
	$(0, \frac{1}{2})$	$(2, \frac{3}{2})$	$(1, \frac{1}{2}+\frac{3}{2})$	$(0, \frac{1}{2})$	$(2, \frac{3}{2})$	$(1, \frac{1}{2}+\frac{3}{2})$
$(0, \frac{1}{2})$	4.09	-22.54	-0.00	9.72	-33.60	-0.03
$(2, \frac{3}{2})$		10.85	-0.23		16.35	-0.42
$(1, \frac{1}{2}+\frac{3}{2})$			0.11			0.22
^{4}He(0_1^+)						
	(0,0)	(2,2)	(1,1)	(0,0)	(2,2)	(1,1)
(0,0)	0.95	-46.65	-0.01	12.94	-68.67	-0.21
(2,2)		21.24	-1.56		32.31	-2.90
(1,1)			0.72			1.47

Table 4. The Hamiltonian matrix elements, given in MeV, for the 0_1^- state of ^{4}He. The column-row of the matrix is labeled by the channel (L, S), which is arranged in the order of $(1, 1)$ and $(2,2)$. See text for the matrix elements in parentheses. The $P(L, S)$ values are $P(1, 1)=0.955$ and $P(2, 2)=0.045$. The G3RS potential is used.

H		T	
0.64	−13.50	41.19 (43.13)	–
	6.46		7.19 (159.7)
V_{c}		V_{Coul}	
−27.82 (−29.13)	–	0.46 (0.48)	–
	−1.10 (−24.42)		0.02 (0.45)
V_{t}		V_{b}	
−13.48 (−14.11)	−13.51 (−65.15)	0.28 (0.30)	0.01 (0.04)
	0.35 (7.81)		−0.00 (−0.00)

trix element of the Hamiltonian is $0.64\,$MeV in $(1, 1)$ channel and $6.46\,$MeV in $(2, 2)$ channel. The unnatural parity channel gives large positive energy because its kinetic energy is very large. However, the coupling matrix element between $(1, 1)$ and $(2, 2)$ channels amounts to $-13.50\,$MeV, which locates the 0_1^- state at $-6.40\,$MeV in good agreement with experiment. This large coupling matrix element is brought about by the tensor force and its contribution is quite significant. The admixture of the unnatural parity components is so large as 4.5%. We repeated a calculation by omitting the $(2, 2)$ channel. The resulting energy is approximately $-1\,$MeV, which is higher by about $5\,$MeV than the full channel calculation. Though the importance of the tensor force in the 0_1^- state was pointed out many years ago [27, 28], the present result indicates that not only the tensor force but also the kinetic energy and the central force are important factors to determine the energy of the 0_1^- state. Our calculation ignores another unnatural parity component $(0, 0)$. However, its contribution is probably negligible because it has no tensor coupling with the main channel $(1, 1)$.

It is interesting to ask the following question: How different are the G3RS and AV8′ potentials? As seen in Table 2, both potentials give similar energies for the few-nucleon systems. Figure 1 displays the energy change of the ground and first excited states of ^{4}He as a function of the basis dimension. Here the basis set is the one selected using the G3RS Hamiltonian. The basis is increased to optimize the 0_2^+ state after the dimension of 400. In the curves labeled G3RS the basis functions are ordered according to the importance criterion for the ground state. Now the curves labeled AV8′ stand for the energy change obtained by just diagonalizing the AV8′ Hamiltonian in the same basis set. The energy obtained in this way loses only $210\,$keV compared to the energy listed in Table 2. This means that the basis set determined with the G3RS potential already provides a fairly good basis set for the AV8′ potential. Thus one may skip the basis search for AV8′ but only needs to fine-tune the basis to reach the converged solution. This is particularly helpful in saving computer time because the G3RS potential is mild and simple enough to render numerical calculations fast.

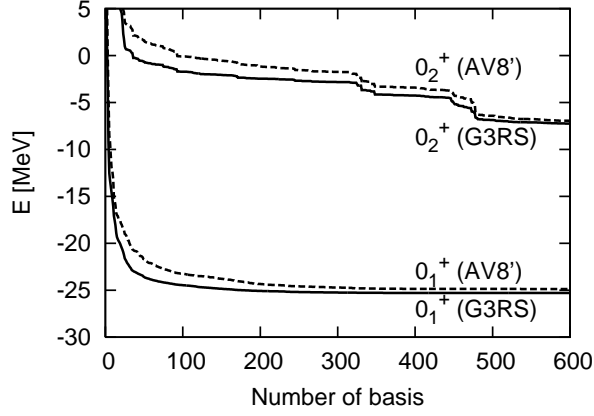Using Eq. (B.26) and noting the remark below it enables one to calculate the

Figure 1. The energy convergence of the ground and first excited states of ^{4}He with the G3RS and AV8$'$ potentials. The basis set is selected for the G3RS potential by the SVM, and the same set is used to calculate the energy with the AV8$'$ potential.

correlation function

$$C(r) = \frac{1}{4\pi r^2} \langle \Psi | \, \delta(|\boldsymbol{r}_1 - \boldsymbol{r}_2| - r) \, | \Psi \rangle, \tag{5.5}$$

which has the normalization of $4\pi \int_0^\infty dr \, r^2 C(r) = 1$. The left panel of Fig. 2 plots the correlation functions of the α-particle calculated with the different potentials. The curve with AV8$'$ agrees very well with that of the benchmark calculation [14]. The curves calculated with the realistic forces show a strong depression at short distances due to the short-ranged repulsion, which is in sharp contrast with the MN potential case. One can see that the AV8$'$ correlation function is more strongly suppressed than that of the G3RS potential. All the correlation functions are similar at large distances. The right panel of Fig. 2 compares the correlation
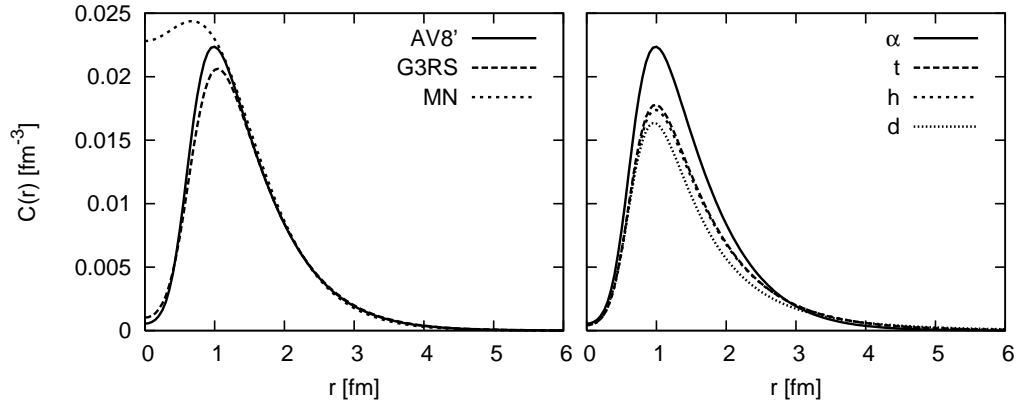
Figure 2. Left: the correlation functions of α-particle with the different potentials. Right: the correlation functions for the ground states of few-nucleon systems calculated with the AV8$'$ potential.

functions for few-nucleon systems calculated with the AV8′ potential. We note that the peak position of $C(r)$ is almost independent of the systems. One can see that the correlation function of the α-particle has larger amplitude around $r=1$ fm and a shorter tail than those of deuteron and ^{3}H.

A two-nucleon momentum distribution also gives useful information on the correlation. The momentum distribution is easily calculated by transforming the coordinate-space wave function to momentum space (see Appendices A and B.3):

$$C(k) = \frac{1}{4\pi k^2} \langle \Psi | \, \delta(\tfrac{1}{2} \, |\boldsymbol{k}_1 - \boldsymbol{k}_2| - k) \{P_{1N} P_{2N}\}_+ \, |\Psi \rangle \,, \qquad (5.6)$$

where the projection operator of a pair of nucleons, $\{P_{1N} P_{2N}\}_+$, stands for

$$\begin{pmatrix} P_{1\pi} P_{2\pi} \\ P_{1\nu} P_{2\nu} \\ \tfrac{1}{2}(P_{1\pi} P_{2\nu} + P_{1\nu} P_{2\pi}) \end{pmatrix} \quad \text{for} \quad \begin{pmatrix} pp \\ nn \\ pn \end{pmatrix}. \qquad (5.7)$$

The momentum distribution defined above has the following normalization

$$4\pi \int_0^\infty dk \, k^2 C(k) = \frac{2}{A(A-1)} \langle \Psi | \sum_{i<j} \{P_{iN} P_{jN}\}_+ |\Psi \rangle. \qquad (5.8)$$

We plot in Fig. 3 the np and pp momentum distributions of the α-particle. The realistic forces produce similar distributions. The distribution calculated with the MN potential follows the realistic distribution up to $k < 1.3$ fm^{-1}, but then decreases rapidly as the momentum increases. This is because the MN potential has neither strong short-ranged repulsion nor tensor force [25]. As shown in ref. [29], both np and pp distributions do not show very different behavior except that the former is roughly four times larger than the latter as expected from the relation (5.8). This is in sharp contrast to a specific momentum distribution such that the sum of the two momenta, $\boldsymbol{k}_1 + \boldsymbol{k}_2$, is close to zero [25, 29], where the nn (pp) momentum distribution, differently from the np distribution, is characterized by a dip around 2 fm^{-1}.
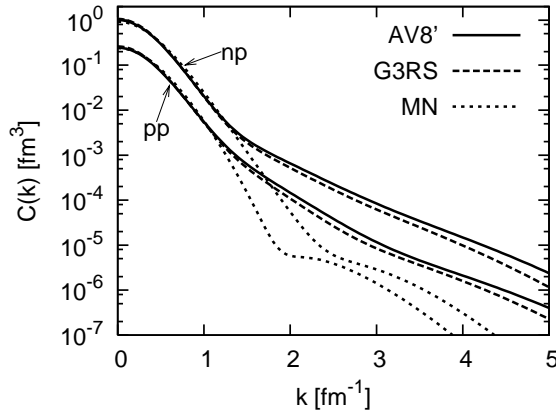

Figure 3. Two-nucleon relative momentum distributions of α-particle with the different potentials.

Calculations for other J^π states of ^{4}He are in progress. A detailed analysis will be reported elsewhere [30].

5.2 3α system with a nonlocal RGM potential

A second test of the CG basis calculation is a 3α system for ^{12}C. That the $\alpha\alpha$ potential cannot be local for describing ^{12}C is not surprising because the interaction between composite particles is intrinsically nonlocal. Such interactions between two composite particles can be derived microscopically within the RGM. A first attempt to use an energy-dependent $\alpha\alpha$ RGM kernel has been developed in ref. [31] in a study of ^{12}C. Using some average energy for this kernel provides fair results for ^{12}C [32] but not for other three-cluster systems [33]. Hence the energy dependence is eliminated from the RGM equation, which enables us to obtain energy-independent nonlocal kernels. Recently, we have shown that this procedure leads to a consistent description of the two 0^+ states of ^{12}C [34] as well as the $3/2^-$ and $5/2^-$ states of ^{9}Be and the ground state of ^{6}He [35].

The RGM equation for the two-cluster relative motion function χ reads

$$(T + V + \varepsilon K)\chi = \varepsilon\chi, \tag{5.9}$$

with a bare RGM potential V

$$V = V_{\mathrm{D}} + V^{\mathrm{EX}} = V_{\mathrm{D}} + K_T + K_V. \tag{5.10}$$

Here T is the intercluster kinetic energy, K is the overlap kernel, V_{D} is local and called the direct potential, and the nonlocal potential V^{EX} comprises K_T and K_V which are the exchange nonlocal kernels for the kinetic and potential (including the Coulomb term) energies, respectively. Equation (5.9) can be converted to an energy-independent equation for $g = \sqrt{\mathcal{N}}\chi = \sqrt{1 - K}\chi$ as follows:

$$(T + V^{\mathrm{RGM}})g = \varepsilon g \tag{5.11}$$

with

$$V^{\mathrm{RGM}} = \mathcal{N}^{-1/2}(T + V)\mathcal{N}^{-1/2} - T = V + W, \tag{5.12}$$

where W is a difference between the renormalized RGM potential V^{RGM} and the bare RGM potential V:

$$W = \mathcal{N}^{-1/2}(T + V)\mathcal{N}^{-1/2} - (T + V). \tag{5.13}$$

The energy-independent potential V^{RGM} serves as an interaction between the composite particles. As shown in ref. [35] the nonlocal interaction W can very well be approximated with $\lambda W^{(1)}$, where

$$W^{(1)} = \frac{1}{2}[K(T + V) + (T + V)K], \tag{5.14}$$

and λ is an appropriate constant. The λ value is set to be 1.30 for the $\alpha\alpha$ case. The $\alpha\alpha$ potential we use in the present study takes the form $V + \lambda W^{(1)}$. All of the needed $\alpha\alpha$ RGM kernels are explicitly given in ref. [33]. We use the harmonic-oscillator parameter $b = 1.36\,\mathrm{fm}$ for the single-nucleon orbit in the α cluster,

and the MN potential [22] with $u = 0.94687$ as the two-nucleon potential. The nonlocal $\alpha\alpha$ potential constructed in this way reproduces the $\alpha\alpha$ phase shifts very well.

To obtain the ground and first excited 0^+ states of ^{12}C, we must have such a solution that does not contain Pauli-forbidden states $\varphi_{n\ell m}$. These states are defined as redundant states of the 2α RGM equation (5.9). They are $0s$, $1s$ and $0d$ harmonic-oscillator states. We define an operator Γ for the 3α system by

$$\Gamma = \sum_{l>k=1}^{3} \Gamma_{kl}, \tag{5.15}$$

where Γ_{kl} is a separable nonlocal operator acting on the relative motion of the particles k and l:

$$\Gamma_{kl} = \Gamma_{kl}(0s) + \Gamma_{kl}(1s) + \Gamma_{kl}(0d) \tag{5.16}$$

with

$$\Gamma_{kl}(n\ell) = \sum_{m=-\ell}^{\ell} | \varphi_{n\ell m}(\boldsymbol{r}_k - \boldsymbol{r}_l)\rangle\langle\varphi_{n\ell m}(\boldsymbol{r}_k - \boldsymbol{r}_l) | . \tag{5.17}$$

Eliminating the forbidden states is performed by adding a pseudopotential $\gamma\Gamma$ to the 3α Hamiltonian and finding such a solution that is stable for sufficiently large γ [36]. In practice, the γ value is set around 10^4 MeV in the present calculation. Since it is hard to eliminate the forbidden states to high accuracy in a nonorthogonal basis set like the CG basis, the use of larger γ values leads to numerically unstable energies. The matrix elements of the nonlocal potentials, V, $W^{(1)}$ and $\Gamma(n\ell)$, can all be calculated using the formulas in Appendices C and D.

Table 5 compares the present result with that obtained by the HH approach [35]. In the HH expansion method the size of the three-body basis depends on the maximum hypermomentum $K_{\max}$. The HH calculation in the table uses $K_{\max} = 36$, and for this value there are 100 HH in the variational expansion of the wave function [37]. Also the hyperradius variable is discretized over 35 points and thus the Hamiltonian matrix has a size of 3500×3500. In contrast to the HH expansion, the solution in the CG approach employs 200 basis functions. The energies of both the 0_1^+ and 0_2^+ states are in good agreement between the two calculations. These values agree reasonably well with the experimental energies. In particular the energy of the 0_2^+ state is in excellent agreement with the observed state called the Hoyle state. The matter rms radius of ^{12}C is defined by adding the empirical value of the α-particle ($\sqrt{\langle r_\alpha^2\rangle} = 1.479$ fm). The radius for the ground state agrees between the two calculations. The comparison of the HH and CG results indicates that the CG basis is quite flexible to describe the different shapes of the wave functions in a small dimension.

The expectation value of each term of the Hamiltonian is also listed in Table 5. It agrees within 30 keV for the 0_1^+ state between the two methods, but the difference is still larger for the 0_2^+ state. This may be due to that both methods obtain the latter state in a bound-state approximation without imposing a proper asymptotic condition, though it is located above the 3α threshold. To judge how well the elimination of the Pauli-forbidden components is achieved with the 200

Table 5. The energy E (MeV) from the 3α threshold and the rms radius $\sqrt{\langle r^2 \rangle}$ (fm) for the ground state and the first excited 0^+ state of ^{12}C. The energy-independent $\alpha\alpha$ RGM potential is used. The expectation value of each piece of the Hamiltonian is also shown. Experimental energies are -7.27 and 0.38 MeV for the 0_1^+ and 0_2^+ states, respectively. The inputs are taken as $\hbar^2/m_N = 41.472$ MeV fm^2, $m_\alpha = 4m_N$, $e^2 = 1.44$ MeV fm^{-2}, where m_α is the mass of α-particle.

Method	L^π	E	$\langle T \rangle$	$\langle V_{\mathrm{D}} \rangle$	$\langle V^{\mathrm{EX}} + \lambda W^{(1)} \rangle$	$\lambda \langle W^{(1)} \rangle$	$\sqrt{\langle r^2 \rangle}$
CG	0_1^+	-9.83	79.06	-80.34	-8.55	7.75	2.19
	0_2^+	0.42	20.34	-18.32	-1.60	0.68	
HH	0_1^+	-9.83	79.09	-80.36	-8.56		2.19
	0_2^+	0.43	21.5	-19.38	-1.69		

basis functions, we show the expectation value of Γ: It is 1.34×10^{-6} for 0_1^+ and 2.19×10^{-7} for 0_2^+, respectively. The contribution from the pseudopotential $\gamma \Gamma$ is subtracted in the energy listed in the table.

As discussed in refs. [36, 34], a local $\alpha\alpha$ potential leads to unphysical results for the 3α energies even though the potential fits the $\alpha\alpha$ phase shifts. For example, the well-known $\alpha\alpha$ potential [38] called the BFW potential gives an extremely deep energy of -19.08 MeV for the 0_1^+ state. This is the main reason why we advocate the importance of using the energy-independent RGM kernel as the interaction between the composite particles. Though the BFW potential cannot produce a physically acceptable result for the 0_1^+ state, it may be worthwhile testing if this potential could be used for setting up a suitable basis set for the 3α Hamiltonian with the nonlocal potential. This is so because the BFW potential whose nuclear part is given by a single Gaussian is by far economical than the nonlocal RGM potential from the point of view of computer time. Figure 4 displays the energy convergence as the basis dimension increases. In this figure the basis set is selected to optimize the 0_1^+ and 0_2^+ states for the 3α Hamiltonian employing the BFW $\alpha\alpha$ potential. This basis set is now just used to diagonalize
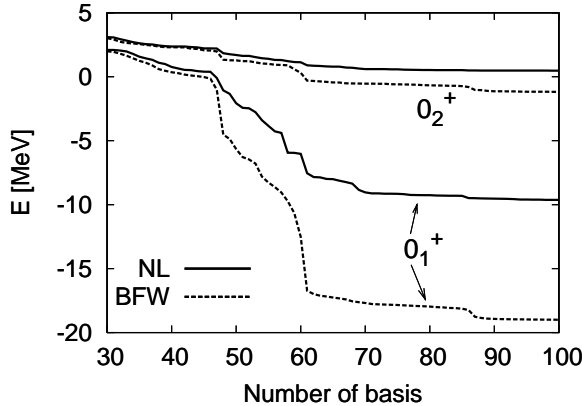

Figure 4. The energy convergence of the 0^+ states of ^{12}C with the BFW and nonlocal RGM (NL) potentials. The basis set is determined by the SVM for the BFW potential.

the Hamiltonian with the nonlocal $\alpha\alpha$ potential. The curves labeled NL display the energy convergence of the latter calculation for the two 0^+ states. The resulting energies are $-9.75\,\text{MeV}$ for the 0_1^+ state and $0.43\,\text{MeV}$ for the 0_2^+ state, which are close to those of Table 5. The rms radius of the 0_1^+ state is reproduced as well. In fact the overlap between the wave functions obtained in the set of Table 5 and the common set noted above is 0.9995 for 0_1^+ and 0.9987 for 0_2^+. This finding is quite appealing for studying a multi-α system interacting via the nonlocal $\alpha\alpha$ potential. We just use the BFW potential to set up a suitable basis set and then use the refinement process to adapt the basis set to the nonlocal potential. This will be much more economical than selecting from the beginning the basis for the Hamiltonian with the nonlocal potential. A calculation along this line is in progress for a 4α description of ^{16}O.

6 Summary

We have extended our previous study on the global vector representation to cope with the orbital motion with an unnatural parity. The basic idea is to introduce two global vectors which are defined by a linear combination of the particle coordinates. Combining these angular parts with a spherical part of the orbital function provides a flexible basis function. We have shown that the matrix elements for most of physical operators of interest including nonlocal operators can be derived analytically if the spherical part is taken as a correlated Gaussian. The fact that its Fourier transform again takes the same functional form opens a wide applicability for studying correlations of a system in momentum space.

Our numerical test examples included $A{=}3$, 4 nuclei interacting via realistic interactions of AV8 type. They have demonstrated the applicability and accuracy of the present method, in comparison with the partial-wave expansion results. We have shown that the 0_1^- state of ^{4}He at the excitation energy of $21.01\,\text{MeV}$ offers a good example to indicate the importance of the tensor coupling between the natural parity and unnatural parity components. The correlated Gaussian basis was also tested for a nonlocal potential in the 3α system, and it succeeded to reproduce the results of the extensive hyperspherical harmonics calculation.

A correlated Gaussian with the global vectors can easily be adapted to bound-state problems of a larger system as the tedious angular momentum couplings of partial-wave expansion are avoided. It will be interesting to devise a method of applying this flexibility to a continuum calculation of scattering and reactions of few-body systems.

Appendix A: Momentum representation of correlated Gaussian basis

The Fourier transform of the CG defines the corresponding basis function in momentum space. As is shown in Eq. (A.7) below, it is again a linear combination of the momentum space CG. The case with a single GV has recently been carried out in ref. [39]. The momentum space CG is useful to evaluate matrix elements such as semi-relativistic kinetic energy or momentum distribution between the particles. See Appendix B.3.

The transformation from the coordinate to momentum space is achieved by a function

$$\Phi(\boldsymbol{k}, \boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{3}{2}(N-1)}}\,\mathrm{e}^{i\tilde{\boldsymbol{k}}\boldsymbol{x}}, \tag{A.1}$$

where $\boldsymbol{k}$ is an $(N-1)$-dimensional column vector whose ith element $\boldsymbol{k}_i$, multiplied by $\hbar$, is a momentum conjugate to $\boldsymbol{x}_i$. The Fourier transform of the generating function g reads

$$\langle\Phi(\boldsymbol{k},\boldsymbol{x})|g(\lambda_1\boldsymbol{e}_1u_1+\lambda_2\boldsymbol{e}_2u_2;A,\boldsymbol{x})\rangle = \frac{1}{(\det A)^{\frac{3}{2}}}\,\mathrm{e}^{\frac{1}{2}\tilde{\boldsymbol{v}}A^{-1}\boldsymbol{v}}, \tag{A.2}$$

where $\boldsymbol{v} = \lambda_1\boldsymbol{e}_1u_1+\lambda_2\boldsymbol{e}_2u_2-i\boldsymbol{k}$. Simplifying $\tilde{\boldsymbol{v}}A^{-1}\boldsymbol{v}$ by omitting both λ_1^2 and λ_2^2 terms, we have

$$\frac{1}{2}\tilde{\boldsymbol{v}}A^{-1}\boldsymbol{v} \longrightarrow \lambda_1\lambda_2\rho\,\boldsymbol{e}_1\cdot\boldsymbol{e}_2 - i\lambda_1\boldsymbol{e}_1\cdot\widetilde{A^{-1}u_1}\boldsymbol{k} - i\lambda_2\boldsymbol{e}_2\cdot\widetilde{A^{-1}u_2}\boldsymbol{k} - \frac{1}{2}\tilde{\boldsymbol{k}}A^{-1}\boldsymbol{k} \tag{A.3}$$

with

$$\rho = \widetilde{u_1}A^{-1}u_2. \tag{A.4}$$

Here the symbol $\longrightarrow$ indicates that the λ_i^2 terms can safely be dropped. Substituting Eqs. (A.2) and (A.3) into Eq. (2.9) enables us to derive

$$\langle\Phi(\boldsymbol{k},\boldsymbol{x})|F_{(L_1L_2)LM}(u_1,u_2,A,\boldsymbol{x})\rangle = B_{L_1}B_{L_2}\frac{1}{(\det A)^{\frac{3}{2}}}\exp\left(-\frac{1}{2}\tilde{\boldsymbol{k}}A^{-1}\boldsymbol{k}\right)$$

$$\times \sum_{\ell=0}^{\min(L_1,L_2)}\frac{(-i)^{L_1+L_2-2\ell}}{\ell!(L_1-\ell)!(L_2-\ell)!}\rho^\ell\int\int d\boldsymbol{e}_1\,d\boldsymbol{e}_2\,[Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)]_{LM}$$

$$\times(\boldsymbol{e}_1\cdot\boldsymbol{e}_2)^\ell(\boldsymbol{e}_1\cdot\widetilde{A^{-1}u_1}\boldsymbol{k})^{L_1-\ell}(\boldsymbol{e}_2\cdot\widetilde{A^{-1}u_2}\boldsymbol{k})^{L_2-\ell}. \tag{A.5}$$

As noted below Eq. (2.10), the above integration has a non-vanishing contribution provided the vectors $\boldsymbol{e}_i$ couple to their maximum value L_i. This can be done using the relation

$$(\boldsymbol{e}_1\cdot\boldsymbol{e}_2)^\ell \Rightarrow \frac{\ell!}{B_\ell}(-1)^\ell\sqrt{2\ell+1}[Y_\ell(\boldsymbol{e}_1)Y_\ell(\boldsymbol{e}_2)]_{00}, \tag{A.6}$$

where the symbol $\Rightarrow$ indicates that the angular momentum coupling must be made to its maximum value for each $\boldsymbol{e}_i$. The terms $(\boldsymbol{e}_1\cdot\widetilde{A^{-1}u_1}\boldsymbol{k})^{L_1-\ell}$ and $(\boldsymbol{e}_2\cdot\widetilde{A^{-1}u_2}\boldsymbol{k})^{L_2-\ell}$ are expanded in a similar manner. Combining these results leads to

$$\langle\Phi(\boldsymbol{k},\boldsymbol{x})|F_{(L_1L_2)LM}(u_1,u_2,A,\boldsymbol{x})\rangle$$

$$= \frac{(-i)^{L_1+L_2}}{(\det A)^{\frac{3}{2}}}\sum_{\ell=0}^{\ell_M}\mathcal{K}(L_1L_2L;\ell)(-\rho)^\ell F_{(L_1-\ell\,L_2-\ell)LM}(A^{-1}u_1,A^{-1}u_2,A^{-1},\boldsymbol{k}), \tag{A.7}$$

where $\ell_M = \min(L_1,L_2,[(L_1+L_2-L)/2])$. The coefficient $\mathcal{K}(L_1L_2L;\ell)$ is given by

$$\mathcal{K}(L_1L_2L;\ell) = \frac{4\pi(-1)^{\ell+L-L_1-L_2}(2L_1+1)!!(2L_2+1)!!}{(2\ell+1)!!(2L_1-2\ell+1)!!(2L_2-2\ell+1)!!}\sqrt{\frac{(2L_1+1)(2L_2+1)}{(2\ell+1)(2L+1)}}$$

$$\times\ C(\ell\,L_1-\ell;L_1)\,C(\ell\,L_2-\ell;L_2)\,U(L_1-\ell\,L_1\,L_2-\ell\,L_2;\ell L), \tag{A.8}$$

where C is a coefficient which couples two spherical harmonics with the same argument

$$C(l_1l_2;l_3) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}}\langle l_10l_20|l_30\rangle, \tag{A.9}$$

and U is a unitary Racah coefficient [9].

The Fourier transforms of the CG of Eqs. (2.4) and (2.6) are particularly simple:

$$\langle\Phi(\boldsymbol{k},\boldsymbol{x})|F_{(L0)LM}(u_1,u_2,A,\boldsymbol{x})\rangle = \frac{(-i)^L}{(\det A)^{\frac{3}{2}}}F_{(L0)LM}(A^{-1}u_1,A^{-1}u_2,A^{-1},\boldsymbol{k}),$$

$$\langle\Phi(\boldsymbol{k},\boldsymbol{x})|F_{(L1)LM}(u_1,u_2,A,\boldsymbol{x})\rangle = \frac{(-i)^{L+1}}{(\det A)^{\frac{3}{2}}}F_{(L1)LM}(A^{-1}u_1,A^{-1}u_2,A^{-1},\boldsymbol{k}). \tag{A.10}$$

Appendix B: Matrix elements of local operators

B.1 Overlap

The overlap matrix element between the generating functions becomes

$$\langle g(\lambda_3 e_3 u_3 + \lambda_4 e_4 u_4; A', \boldsymbol{x}) | g(\lambda_1 e_1 u_1 + \lambda_2 e_2 u_2; A, \boldsymbol{x}) \rangle = \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \exp\left(\frac{1}{2} \tilde{\boldsymbol{v}} B^{-1} \boldsymbol{v} \right)$$

$$\longrightarrow \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \exp\left(\sum_{j>i=1}^{4} \rho_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right), \tag{B.1}$$

where

$$\boldsymbol{v} = \sum_{i=1}^{4} \lambda_i \boldsymbol{e}_i u_i, \tag{B.2}$$

and

$$B = A + A', \qquad \rho_{ij} = \widetilde{u}_i B^{-1} u_j. \tag{B.3}$$

Following the procedure explained in Section (3) and using Eq. (A.6), we have

$$\prod_{j>i=1}^{4} \frac{(\rho_{ij} \boldsymbol{e}_i \cdot \boldsymbol{e}_j)^{p_{ij}}}{p_{ij}!} \Rightarrow \left(\prod_{j>i=1}^{4} \frac{(-1)^{p_{ij}} \sqrt{2p_{ij}+1}}{B_{p_{ij}}} (\rho_{ij})^{p_{ij}} \right) \sum_{L} X(p_{13} p_{14} p_{23} p_{24}; L)$$

$$\times Y(p_{12} p_{12} p_{34} p_{34} L_1 - p_{12} L_2 - p_{12} L_3 - p_{34} L_4 - p_{34} 0 L L 0; L L)$$

$$\times \left[[Y_{L_1}(\boldsymbol{e}_1) Y_{L_2}(\boldsymbol{e}_2)]_L [Y_{L_3}(\boldsymbol{e}_3) Y_{L_4}(\boldsymbol{e}_4)]_L \right]_{00}. \tag{B.4}$$

Here the non-negative integer powers p_{ij} are restricted by L_i as follows:

$$p_{12} + p_{13} + p_{14} = L_1, \quad p_{12} + p_{23} + p_{24} = L_2,$$
$$p_{13} + p_{23} + p_{34} = L_3, \quad p_{14} + p_{24} + p_{34} = L_4. \tag{B.5}$$

The coefficient X needed for a stretched coupling for each $\boldsymbol{e}_i$,

$$[Y_a(\boldsymbol{e}_1) Y_a(\boldsymbol{e}_3)]_{00} [Y_b(\boldsymbol{e}_1) Y_b(\boldsymbol{e}_4)]_{00} [Y_c(\boldsymbol{e}_2) Y_c(\boldsymbol{e}_3)]_{00} [Y_d(\boldsymbol{e}_2) Y_d(\boldsymbol{e}_4)]_{00}$$

$$\Rightarrow \sum_{L} X(abcd; L) \left[[Y_{a+b}(\boldsymbol{e}_1) Y_{c+d}(\boldsymbol{e}_2)]_L [Y_{a+c}(\boldsymbol{e}_3) Y_{b+d}(\boldsymbol{e}_4)]_L \right]_{00}, \tag{B.6}$$

is given by

$$X(abcd; L) = \sqrt{\frac{2L+1}{(2a+1)(2b+1)(2c+1)(2d+1)}} \, C(a\,b; a+b) \, C(c\,d; c+d)$$

$$\times \; C(a\,c; a+c) \, C(b\,d; b+d) \begin{bmatrix} a & b & a+b \\ c & d & c+d \\ a+c & b+d & L \end{bmatrix}, \tag{B.7}$$

where the square bracket $[\cdots]$ stands for a unitary 9-j coefficient [9], while the coefficient Y appearing for the coupling

$$\left[\left[[Y_a(\boldsymbol{e}_1) Y_b(\boldsymbol{e}_2)]_\ell [Y_c(\boldsymbol{e}_3) Y_d(\boldsymbol{e}_4)]_\ell \right]_0 \left[[Y_\alpha(\boldsymbol{e}_1) Y_\beta(\boldsymbol{e}_2)]_\lambda [Y_\gamma(\boldsymbol{e}_3) Y_\delta(\boldsymbol{e}_4)]_\nu \right]_\kappa \right]_{\kappa\mu}$$

$$\Rightarrow \sum_{LL'} Y(abcd\alpha\beta\gamma\delta\ell\lambda\nu\kappa; LL') \left[[Y_{a+\alpha}(\boldsymbol{e}_1) Y_{b+\beta}(\boldsymbol{e}_2)]_L [Y_{c+\gamma}(\boldsymbol{e}_3) Y_{d+\delta}(\boldsymbol{e}_4)]_{L'} \right]_{\kappa\mu}, \tag{B.8}$$

is given by

$$Y(abcd\alpha\beta\gamma\delta\ell\lambda\nu\kappa; LL') = \begin{bmatrix} \ell & \ell & 0 \\ \lambda & \nu & \kappa \\ L & L' & \kappa \end{bmatrix} \begin{bmatrix} a & b & \ell \\ \alpha & \beta & \lambda \\ a+\alpha & b+\beta & L \end{bmatrix} \begin{bmatrix} c & d & \ell \\ \gamma & \delta & \nu \\ c+\gamma & d+\delta & L' \end{bmatrix}$$

$$\times \; C(a\alpha; a+\alpha) \, C(b\beta; b+\beta) \, C(c\gamma; c+\gamma) \, C(d\delta; d+\delta). \tag{B.9}$$

The overlap matrix element reads

$$\langle F_{(L_3L_4)LM}(u_3, u_4, A', \boldsymbol{x})|F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \frac{(-1)^{L_1+L_2}}{\sqrt{2L+1}} \left(\prod_{i=1}^4 B_{L_i}\right) \left(\frac{(2\pi)^{N-1}}{\det B}\right)^{\frac{3}{2}} \sum_{p_{ij}} \left(\prod_{j>i=1}^4 \frac{(-1)^{p_{ij}}\sqrt{2p_{ij}+1}}{B_{p_{ij}}}(\rho_{ij})^{p_{ij}}\right) \quad \text{(B.10)}$$

$$\times X(p_{13}p_{14}p_{23}p_{24}; L)Y(p_{12}p_{12}p_{34}p_{34} \, L_1-p_{12} \, L_2-p_{12} \, L_3-p_{34} \, L_4-p_{34} \, 0LL0; LL).$$

As seen from Eq. (B.5), only two of p_{ij}, e.g., p_{12} and p_{13} are independent for given L_i values. The sum in Eq. (B.10) consists of only few terms: just one term with $p_{13} = L$ for the natural parity, and three terms with (i) $p_{13} = L-1$, $p_{14} = p_{23} = 1$, (ii) $p_{13} = L-1$, $p_{12} = p_{34} = 1$, (iii) $p_{13} = L$, $p_{24} = 1$ for the unnatural parity. Other p_{ij} values all vanish.

B.2 Kinetic energy and mean square distance

The kinetic energy with the center of mass kinetic energy being subtracted is expressed as $T-T_{\rm cm} = (1/2)\widetilde{\boldsymbol{\pi}}\Lambda\boldsymbol{\pi}$, where $\boldsymbol{\pi}_j$ is $-i\hbar\partial/\partial\boldsymbol{x}_j$ and Λ is an appropriate $(N-1)\times(N-1)$ symmetric matrix. The matrix element between the generating functions is given by

$$\langle g(\lambda_3\boldsymbol{e}_3u_3+\lambda_4\boldsymbol{e}_4u_4; A', \boldsymbol{x})|\frac{1}{2}\widetilde{\boldsymbol{\pi}}\Lambda\boldsymbol{\pi}|g(\lambda_1\boldsymbol{e}_1u_1+\lambda_2\boldsymbol{e}_2u_2; A, \boldsymbol{x})\rangle$$

$$= \frac{\hbar^2}{2}(R - \widetilde{\boldsymbol{z}}\Lambda\boldsymbol{z}) \left(\frac{(2\pi)^{N-1}}{\det B}\right)^{\frac{3}{2}} \exp\left(\frac{1}{2}\widetilde{\boldsymbol{v}}B^{-1}\boldsymbol{v}\right), \quad \text{(B.11)}$$

where

$$\boldsymbol{z} = \sum_{i=1}^4 \lambda_i\boldsymbol{e}_iA_iB^{-1}u_i, \qquad R = 3\text{Tr}(B^{-1}A'\Lambda A), \quad \text{(B.12)}$$

with

$$A_1 = A_2 = A', \qquad A_3 = A_4 = -A. \quad \text{(B.13)}$$

The desired matrix element is expressed using the overlap matrix element as follows:

$$\langle F_{(L_3L_4)LM}(u_3, u_4, A', \boldsymbol{x})|T - T_{\rm cm}|F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \frac{\hbar^2}{2}\left(R - 2\sum_{j>i=1}^4 S_{ij}\frac{\partial}{\partial\rho_{ij}}\right)\langle F_{(L_3L_4)LM}(u_3, u_4, A', \boldsymbol{x})|F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle, \text{(B.14)}$$

where

$$S_{ij} = \widetilde{u_i}B^{-1}A_i\Lambda A_jB^{-1}u_j. \quad \text{(B.15)}$$

Since ρ_{ij} appears only as $(\rho_{ij})^{p_{ij}}$ in $\langle F'|F\rangle$, its differentiation is elementary.

A mean square distance is a quantity to characterize the size of a system. What is meant by it is the expectation value of an operator such as $(\boldsymbol{r}_k-\boldsymbol{r}_l)^2$ or $\sum_{k=1}^N(\boldsymbol{r}_k-\boldsymbol{x}_N)^2$. Clearly such operators can be expressed as $\widetilde{\boldsymbol{x}}Q\boldsymbol{x}$ with an appropriate symmetric matrix Q. For example, Eq. (4.1) enables us to obtain $Q = w\widetilde{w}$ for the case of $(\boldsymbol{r}_k-\boldsymbol{r}_l)^2$. The matrix element of $\widetilde{\boldsymbol{x}}Q\boldsymbol{x}$ between the generating functions takes the form

$$\langle g(\lambda_3\boldsymbol{e}_3u_3+\lambda_4\boldsymbol{e}_4u_4; A', \boldsymbol{x})|\widetilde{\boldsymbol{x}}Q\boldsymbol{x}|g(\lambda_1\boldsymbol{e}_1u_1+\lambda_2\boldsymbol{e}_2u_2; A, \boldsymbol{x})\rangle$$

$$= (\mathcal{R} + \widetilde{\boldsymbol{v}}B^{-1}QB^{-1}\boldsymbol{v}) \left(\frac{(2\pi)^{N-1}}{\det B}\right)^{\frac{3}{2}} \exp\left(\frac{1}{2}\widetilde{\boldsymbol{v}}B^{-1}\boldsymbol{v}\right) \quad \text{(B.16)}$$

with $\mathcal{R} = 3\text{Tr}(B^{-1}Q)$. Comparing to the kinetic energy matrix element (B.11) leads to

$$\langle F_{(L_3L_4)LM}(u_3, u_4, A', \boldsymbol{x})|\widetilde{\boldsymbol{x}}Q\boldsymbol{x}|F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \left(\mathcal{R} + 2\sum_{j>i=1}^4 \mathcal{S}_{ij}\frac{\partial}{\partial\rho_{ij}}\right)\langle F_{(L_3L_4)LM}(u_3, u_4, A', \boldsymbol{x})|F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle \quad \text{(B.17)}$$

with $\mathcal{S}_{ij} = \widetilde{u_i}B^{-1}QB^{-1}u_j$.

B.3 δ-function or multipole operator

A local potential $V(\boldsymbol{r}_k - \boldsymbol{r}_l)$ can be expressed with use of $\boldsymbol{r}_k - \boldsymbol{r}_l = \widetilde{w}\boldsymbol{x}$ (see Eq. (4.1)) as

$$V(\boldsymbol{r}_k - \boldsymbol{r}_l) = \int d\boldsymbol{r} V(\boldsymbol{r})\delta(\widetilde{w}\boldsymbol{x} - \boldsymbol{r}). \tag{B.18}$$

The matrix element of V can thus be obtained through that of the δ-function. The single-particle coordinate from the center of mass, $\boldsymbol{r}_k - \boldsymbol{x}_N$, is also expressed in terms of $\boldsymbol{x}_i$ with appropriate coefficients w_i, and a single-particle operator $D(\boldsymbol{r}_k - \boldsymbol{x}_N)$ is represented by the δ-function as

$$D(\boldsymbol{r}_k - \boldsymbol{x}_N) = \int d\boldsymbol{r} D(\boldsymbol{r})\delta(\widetilde{w}\boldsymbol{x} - \boldsymbol{r}), \tag{B.19}$$

so that its matrix element again reduces to that of the δ-function.

The matrix element of the δ-function between the generating functions is given by

$$\langle g(\lambda_3\boldsymbol{e}_3 u_3 + \lambda_4\boldsymbol{e}_4 u_4; A', \boldsymbol{x})|\delta(\widetilde{w}\boldsymbol{x} - \boldsymbol{r})|g(\lambda_1\boldsymbol{e}_1 u_1 + \lambda_2\boldsymbol{e}_2 u_2; A, \boldsymbol{x})\rangle$$

$$= \left(\frac{(2\pi)^{N-2}c}{\det B}\right)^{\frac{3}{2}} \exp\left(\frac{1}{2}\widetilde{\boldsymbol{v}}B^{-1}\boldsymbol{v} - \frac{1}{2}c(\boldsymbol{r} - \widetilde{w}B^{-1}\boldsymbol{v})^2\right)$$

$$\longrightarrow \left(\frac{(2\pi)^{N-2}c}{\det B}\right)^{\frac{3}{2}} \exp\left(-\frac{1}{2}cr^2 + \sum_{j>i=1}^{4}\bar{\rho}_{ij}\lambda_i\lambda_j\boldsymbol{e}_i\cdot\boldsymbol{e}_j + c\sum_{i=1}^{4}\gamma_i\lambda_i\boldsymbol{e}_i\cdot\boldsymbol{r}\right), \tag{B.20}$$

where

$$c = (\widetilde{w}B^{-1}w)^{-1}, \qquad \gamma_i = \widetilde{u}_i B^{-1}w = \widetilde{w}B^{-1}u_i, \qquad \bar{\rho}_{ij} = \rho_{ij} - c\gamma_i\gamma_j = \widetilde{u}_i J^{-1}u_j. \tag{B.21}$$

The exponential part including $\boldsymbol{r}$ can be expanded in power series:

$$\prod_{i=1}^{4}\frac{(c\gamma_i\boldsymbol{e}_i\cdot\boldsymbol{r})^{q_i}}{q_i!} \Rightarrow \prod_{i=1}^{4}\frac{(-1)^{q_i}\sqrt{2q_i+1}}{B_{q_i}}(c\gamma_i)^{q_i}r^{q_i}\left[Y_{q_i}(\boldsymbol{e}_i)Y_{q_i}(\hat{\boldsymbol{r}})\right]_{00}$$

$$= \left(\prod_{i=1}^{4}\frac{(-1)^{q_i}(c\gamma_i)^{q_i}}{B_{q_i}}r^{q_i}\right)\sum_{\mu\mu'\ell}\sqrt{2\ell+1}\,C(q_1q_2;\mu)\,C(q_3q_4;\mu')\,C(\mu\mu';\ell)$$

$$\times \left[\left[[Y_{q_1}(\boldsymbol{e}_1)Y_{q_2}(\boldsymbol{e}_2)]_\mu[Y_{q_3}(\boldsymbol{e}_3)Y_{q_4}(\boldsymbol{e}_4)]_{\mu'}\right]_\ell Y_\ell(\hat{\boldsymbol{r}})\right]_{00}. \tag{B.22}$$

Using Eqs. (B.4), (B.8) and (B.22) leads to the formula for the desired matrix element

$$\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x})|\delta(\widetilde{w}\boldsymbol{x} - \boldsymbol{r})|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \frac{(-1)^{L_1+L_2+L+M+L'+M'}}{\sqrt{2L'+1}}\left(\prod_{i=1}^{4}B_{L_i}\right)\left(\frac{(2\pi)^{N-2}c}{\det B}\right)^{\frac{3}{2}}$$

$$\times \sum_{p_{ij}}\left(\prod_{j>i=1}^{4}\frac{(-1)^{p_{ij}}\sqrt{2p_{ij}+1}}{B_{p_{ij}}}(\bar{\rho}_{ij})^{p_{ij}}\right)\sum_{q_i}\left(\prod_{i=1}^{4}\frac{(-1)^{q_i}}{B_{q_i}}(c\gamma_i)^{q_i}\right)$$

$$\times \sum_{\kappa\mu\mu'\ell m}\langle LM\ell m|L'M'\rangle\sqrt{2\ell+1}X(p_{13}p_{14}p_{23}p_{24};\kappa)$$

$$\times Y(p_{12}p_{12}p_{34}p_{34}\ p_{13}+p_{14}\ p_{23}+p_{24}\ p_{13}+p_{23}\ p_{14}+p_{24}\ 0\kappa\kappa0;\kappa\kappa)$$

$$\times Y(L_1-q_1\ L_2-q_2\ L_3-q_3\ L_4-q_4\ q_1q_2q_3q_4\kappa\mu\mu'\ell;LL')$$

$$\times C(q_1q_2;\mu)\,C(q_3q_4;\mu')\,C(\mu\mu';\ell)\,r^{q_1+q_2+q_3+q_4}e^{-\frac{1}{2}cr^2}Y_{\ell\,-m}(\hat{\boldsymbol{r}}). \tag{B.23}$$

Here p_{ij} and q_i are non-negative integers, which must satisfy the following equations

$$p_{12} + p_{13} + p_{14} + q_1 = L_1, \quad p_{12} + p_{23} + p_{24} + q_2 = L_2,$$
$$p_{13} + p_{23} + p_{34} + q_3 = L_3, \quad p_{14} + p_{24} + p_{34} + q_4 = L_4. \tag{B.24}$$

Using the expansion

$$\delta(\widetilde{w}\boldsymbol{x} - \boldsymbol{r}) = \frac{\delta(|\,\widetilde{w}\boldsymbol{x}\,| - r)}{r^2}\sum_{\ell m}Y_{\ell m}(\widehat{\widetilde{w}\boldsymbol{x}})Y_{\ell m}(\hat{\boldsymbol{r}})^*, \tag{B.25}$$

we obtain the matrix element for the multipole operator

$$\langle F_{(L_3 L_4) L' M'}(u_3, u_4, A', \boldsymbol{x}) | V(|\widetilde{w}\boldsymbol{x}|) Y_{\ell m}(\widehat{\widetilde{w}\boldsymbol{x}}) | F_{(L_1 L_2) L M}(u_1, u_2, A, \boldsymbol{x}) \rangle$$

$$= \frac{(-1)^{L_1 + L_2 + L + L'}}{\sqrt{2L'+1}} \langle L M \ell m | L' M' \rangle \sqrt{2\ell+1} \left(\prod_{i=1}^{4} B_{L_i} \right) \left(\frac{(2\pi)^{N-2} c}{\det B} \right)^{\frac{3}{2}}$$

$$\times \sum_{p_{ij}} \left(\prod_{j>i=1}^{4} \frac{(-1)^{p_{ij}} \sqrt{2p_{ij}+1}}{B_{p_{ij}}} (\bar{\rho}_{ij})^{p_{ij}} \right) \sum_{q_i} \left(\prod_{i=1}^{4} \frac{(-1)^{q_i}}{B_{q_i}} (c\gamma_i)^{q_i} \right)$$

$$\times \int_0^{\infty} dr \, r^{q_1 + q_2 + q_3 + q_4 + 2} e^{-\frac{1}{2}cr^2} V(r)$$

$$\times \sum_{\kappa \mu \mu'} X(p_{13} p_{14} p_{23} p_{24}; \kappa) \, C(q_1 q_2; \mu) \, C(q_3 q_4; \mu') \, C(\mu \mu'; \ell)$$

$$\times Y(p_{12} p_{12} p_{34} p_{34} \; p_{13}{+}p_{14} \; p_{23}{+}p_{24} \; p_{13}{+}p_{23} \; p_{14}{+}p_{24} \; 0\kappa\kappa0; \kappa\kappa)$$

$$\times Y(L_1{-}q_1 \; L_2{-}q_2 \; L_3{-}q_3 \; L_4{-}q_4 \; q_1 q_2 q_3 q_4 \kappa \mu \mu' \ell; L L'). \tag{B.26}$$

Equation (B.26) with $\ell m = 00$ has many important applications. The matrix element of the relative distance $|\boldsymbol{r}_k - \boldsymbol{r}_l|$ or $|\boldsymbol{r}_k - \boldsymbol{x}_N|$ is calculated by choosing $V(r) = r$ with appropriate w. The correlation function (5.5) is also easily calculated by choosing $V(r) = \delta(r - a)$ (with a being replaced by r later). Of particular importance in hadron spectroscopy is the matrix element for the semi-relativistic kinetic energy, $\sqrt{(\widetilde{w}\boldsymbol{\pi})^2 + \mu^2}$. This matrix element reduces to that of the central matrix element with $V(r) = \sqrt{r^2 + \mu^2}$ because the Fourier transform of the coordinate space CG is expressed in terms of the momentum space CG (see Eq. (A.7)). The relative momentum distribution between the particles (5.6) can also easily be calculated in the momentum space by choosing $V(r)$ appropriately.

The spin-orbit matrix element is obtained from the following result

$$\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) | \delta(\widetilde{w}\boldsymbol{x} - \boldsymbol{r})(\widetilde{w}\boldsymbol{x} \times \widetilde{\xi}\boldsymbol{\pi}) | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle$$

$$= \frac{\hbar}{i} \left(\frac{(2\pi)^{N-2} c}{\det B} \right)^{\frac{3}{2}} \boldsymbol{r} \times (\widetilde{\xi}\boldsymbol{z} + c\widetilde{\xi} A B^{-1} w \widetilde{w} B^{-1} \boldsymbol{v})$$

$$\times \exp \left(\frac{1}{2} \widetilde{\boldsymbol{v}} B^{-1} \boldsymbol{v} - \frac{1}{2} c(\boldsymbol{r} - \widetilde{w} B^{-1} \boldsymbol{v})^2 \right), \tag{B.27}$$

where $\boldsymbol{z}$ is defined in Eq. (B.12). When the radial form of the spin-orbit potential is scalar, i.e. $V(\boldsymbol{r})$ is a function of r, we may omit $c\widetilde{\xi} A B^{-1} w \widetilde{w} B^{-1} \boldsymbol{v}$ thanks to the relation

$$\int d\boldsymbol{r} \, V(r)(\boldsymbol{r} \times \boldsymbol{a}) \exp \left(-\frac{1}{2} c(\boldsymbol{r} - \boldsymbol{a})^2 \right) = 0, \tag{B.28}$$

which leads to

$$\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) | V(|\widetilde{w}\boldsymbol{x}|)(\widetilde{w}\boldsymbol{x} \times \widetilde{\xi}\boldsymbol{\pi})_m | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle$$

$$\longrightarrow \frac{\hbar}{i} \left(\frac{(2\pi)^{N-2} c}{\det B} \right)^{\frac{3}{2}} \int d\boldsymbol{r} \, V(r)(\boldsymbol{r} \times \widetilde{\xi}\boldsymbol{z})_m$$

$$\times \exp \left(-\frac{1}{2} cr^2 + \sum_{j>i=1}^{4} \bar{\rho}_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j + c \sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i \cdot \boldsymbol{r} \right), \tag{B.29}$$

where $(\boldsymbol{a} \times \boldsymbol{b})_m$ stands for $-\sqrt{2}i[\boldsymbol{a} \times \boldsymbol{b}]_{1m} = -(4\sqrt{2}\pi/3)iab[Y_1(\hat{\boldsymbol{a}})Y_1(\hat{\boldsymbol{b}})]_{1m}$.

Comparing Eq. (B.29) with the matrix element (B.20) for the δ-function, it is possible to obtain an analytic expression for the spin-orbit matrix element though it is very much involved.

B.4 Potentials of Gaussian radial form

When the radial form of $V(r)$ is Gaussian, $\exp(-c'r^2/2)$, the formula turns out to be much more concise. Even when its form is not Gaussian, it may be approximated very well by a superposition of Gaussians with different c' values. As we show below, the matrix element of operators with Gaussian radial form can be expressed using the overlap matrix element.

<u>(i) Central potential</u>

Using Eq. (B.20) yields

$$\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x})| \exp\left\{-\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2\right\} |g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x})\rangle$$

$$\longrightarrow \left(\frac{c}{c+c'}\right)^{\frac{3}{2}} \left(\frac{(2\pi)^{N-1}}{\det B}\right)^{\frac{3}{2}} \exp\left(\sum_{j>i=1}^{4} \left[\rho_{ij} - \frac{cc'}{c+c'}\gamma_i\gamma_j\right]\lambda_i\lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j\right). \quad \text{(B.30)}$$

Comparing this result with Eq. (B.1) confirms that ρ_{ij} in the overlap is here replaced with $\rho_{ij} - (cc'/(c+c'))\gamma_i\gamma_j$. The desired matrix element takes exactly the same form as the overlap

$$\langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})| \exp\left\{-\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2\right\} |F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \left(\frac{c}{c+c'}\right)^{\frac{3}{2}} \langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle\Big|_{\rho_{ij} \to \rho_{ij} - \frac{cc'}{c+c'}\gamma_i\gamma_j}. \quad \text{(B.31)}$$

The Coulomb potential $V(r) = 1/r$ is expressed as a superposition of Gaussian potentials:

$$\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_0^\infty dt\, e^{-r^2 t^2}. \quad \text{(B.32)}$$

Thus we obtain

$$\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x})| \frac{1}{|\widetilde{w}\boldsymbol{x}|} |g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x})\rangle$$

$$= \frac{2}{\sqrt{\pi}} \int_0^\infty dt\, \langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x})| \exp\left\{-t^2(\widetilde{w}\boldsymbol{x})^2\right\} |g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x})\rangle$$

$$\longrightarrow \sqrt{\frac{2c}{\pi}} \int_0^1 du \left(\frac{(2\pi)^{N-1}}{\det B}\right)^{\frac{3}{2}} \exp\left(\sum_{j>i=1}^{4} \left[\rho_{ij} - cu^2\gamma_i\gamma_j\right]\lambda_i\lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j\right), \quad \text{(B.33)}$$

where a change of the integration variable is performed through $t = \sqrt{c/2}\, u/\sqrt{1-u^2}$. The Coulomb matrix element reduces to the following integral of the overlap matrix element

$$\langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})| \frac{1}{|\widetilde{w}\boldsymbol{x}|} |F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \sqrt{\frac{2c}{\pi}} \int_0^1 du\, \langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle\Big|_{\rho_{ij} \to \rho_{ij} - cu^2\gamma_i\gamma_j}. \quad \text{(B.34)}$$

The above integrand is a polynomial function of u whose degree is at most $L_1 + L_2 + L_3 + L_4$, so that the integration can be accurately performed with use of the Gauss quadrature.

We note that the modified Coulomb potential

$$\frac{1}{r} \text{erf}(\kappa r) = \frac{2\kappa}{\sqrt{\pi}} \int_0^1 dt\, e^{-\kappa^2 r^2 t^2} \quad \text{(B.35)}$$

can easily be calculated in the same way as above.

Evaluating the matrix element of Yukawa potential is possible with use of Eq. (B.26). Another simple formula is, however, obtained as below. Expressing the Yukawa potential as

$$\frac{1}{r} e^{-\kappa r} = \frac{2}{\sqrt{\pi}} \int_0^\infty dt\, \exp\left(-r^2 t^2 - \frac{\kappa^2}{4t^2}\right), \quad \text{(B.36)}$$

which is a superposition of Gaussian potentials, we get an expression for the matrix element

$$\langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})| \frac{1}{|\widetilde{w}\boldsymbol{x}|} e^{-\kappa|\widetilde{w}\boldsymbol{x}|} |F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \sqrt{\frac{2c}{\pi}} \int_0^1 du\, \exp\left(-\frac{\kappa^2}{2c}\frac{1-u^2}{u^2}\right)$$

$$\times \langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle\Big|_{\rho_{ij} \to \rho_{ij} - cu^2\gamma_i\gamma_j}. \quad \text{(B.37)}$$

As the last example of the Gaussian central potential, we consider $V(r) = r\exp(-c'r^2/2)$, which is a derivative of the Gaussian potential, $\exp(-c'r^2/2)$. Though we can evaluate the matrix element for this potential from Eq. (B.26), it is possible to relate its matrix element to the overlap matrix element. Starting from Eq. (B.20), we obtain

$$
\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) \| \widetilde{w}\boldsymbol{x} | \exp\left\{ -\frac{1}{2} c'(\widetilde{w}\boldsymbol{x})^2 \right\} | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle
$$

$$
\longrightarrow \sqrt{\frac{2}{\pi c}} \left(\frac{c}{c+c'} \right)^2 \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \exp\left(\sum_{j>i=1}^{4} \bar{\rho}_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right)
$$

$$
\times \left(1 + \left[1 + \frac{2c^2}{c+c'} \sum_{j>i=1}^{4} \gamma_i \gamma_j \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right] \right.
$$

$$
\left. \times \int_0^1 du \exp\left\{ \frac{c^2}{c+c'}(1-u^2) \sum_{j>i=1}^{4} \gamma_i \gamma_j \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right\} \right). \tag{B.38}
$$

The required matrix thus reads

$$
\langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x}) | \, |\widetilde{w}\boldsymbol{x}| \, \exp\left\{ -\frac{1}{2} c'(\widetilde{w}\boldsymbol{x})^2 \right\} | F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle
$$

$$
= \sqrt{\frac{2}{\pi c}} \left(\frac{c}{c+c'} \right)^2 \left(\langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x}) | F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle \Big|_{\rho_{ij} \to \bar{\rho}_{ij}} \right.
$$

$$
+ \int_0^1 du \left[1 + \frac{2c^2}{c+c'} \sum_{j>i=1}^{4} \gamma_i \gamma_j \frac{\partial}{\partial \rho_{ij}} \right]
$$

$$
\left. \times \langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x}) | F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle \Big|_{\rho_{ij} \to \rho_{ij} - \frac{c(c'+cu^2)}{c+c'} \gamma_i \gamma_j} \right). \tag{B.39}
$$

(ii) Tensor potential

For $V(\boldsymbol{r}) = \exp\left(-c'r^2/2 \right) Y_{2m}(\hat{\boldsymbol{r}})$, we express it as Gaussian radial form by using a formula

$$
\mathrm{e}^{-\frac{1}{2}c'r^2} Y_{2m}(\hat{\boldsymbol{r}}) = \mathrm{e}^{-\frac{1}{2}c'r^2} \mathcal{Y}_{2m}(\boldsymbol{r}) \int_0^\infty dt \, \mathrm{e}^{-tr^2}. \tag{B.40}
$$

Then use of Eq. (B.20) leads to

$$
\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) | \exp\left\{ -\frac{1}{2} c'(\widetilde{w}\boldsymbol{x})^2 \right\} Y_{2m}(\widehat{\widetilde{w}\boldsymbol{x}}) | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle
$$

$$
\longrightarrow \int_0^\infty dt \int d\boldsymbol{r} \, \mathrm{e}^{-\frac{1}{2}(c'+2t)r^2} \mathcal{Y}_{2m}(\boldsymbol{r})
$$

$$
\times \left(\frac{(2\pi)^{N-2}c}{\det B} \right)^{\frac{3}{2}} \exp\left(-\frac{1}{2}cr^2 + \sum_{j>i=1}^{4} \bar{\rho}_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j + c\sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i \cdot \boldsymbol{r} \right)
$$

$$
\longrightarrow \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \mathcal{Y}_{2m}\left(\sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i \right)
$$

$$
\times \int_0^\infty dt \left(\frac{c}{c+c'+2t} \right)^{\frac{7}{2}} \exp\left(\sum_{j>i=1}^{4} \left[\bar{\rho}_{ij} + \frac{c^2}{c+c'+2t} \gamma_i \gamma_j \right] \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right)
$$

$$
= \frac{c}{2} \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \mathcal{Y}_{2m}\left(\sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i \right)
$$

$$
\times \int_0^{\frac{c}{c+c'}} du \, u^{\frac{3}{2}} \exp\left(\sum_{j>i=1}^{4} \left[\bar{\rho}_{ij} + cu\gamma_i \gamma_j \right] \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right). \tag{B.41}
$$

The term $\mathcal{Y}_{2m}(\sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i)$ is expanded as follows:

$$
\mathcal{Y}_{2m}\left(\sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i \right) = \sum_{i=1}^{4} \gamma_i^2 \lambda_i^2 Y_{2m}(\boldsymbol{e}_i) + \sqrt{\frac{40\pi}{3}} \sum_{j>i=1}^{4} \gamma_i \gamma_j \lambda_i \lambda_j [Y_1(\boldsymbol{e}_i) Y_1(\boldsymbol{e}_j)]_{2m}. \tag{B.42}
$$

The exponential part of the integrand of Eq. (B.41) is expanded in power series $(\lambda_i\lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j)^{\bar{p}_{ij}}$ as in Appendix B.1. Suppose that the $\bar{p}_{ij}$ values give the following angular momenta

$$\bar{p}_{12} + \bar{p}_{13} + \bar{p}_{14} = \bar{L}_1, \quad \bar{p}_{12} + \bar{p}_{23} + \bar{p}_{24} = \bar{L}_2,$$
$$\bar{p}_{13} + \bar{p}_{23} + \bar{p}_{34} = \bar{L}_3, \quad \bar{p}_{14} + \bar{p}_{24} + \bar{p}_{34} = \bar{L}_4. \tag{B.43}$$

These terms contribute to the matrix element provided $\bar{L}_k = L_k - 2\delta_{ki}$ is met in the case of the coupling with $Y_{2m}(\boldsymbol{e}_i)$, the first term of the right side of Eq. (B.42), while $\bar{L}_k = L_k - \delta_{ki} - \delta_{kj}$ is met for the coupling with the second term, $[Y_1(\boldsymbol{e}_i)Y_1(\boldsymbol{e}_j)]_{2m}$. Let us define the corresponding coupling coefficients Z_1 and Z_2 by

$$Y_{\kappa\mu}(\boldsymbol{e}_i)\Big[\big[Y_{\bar{L}_1}(\boldsymbol{e}_1)Y_{\bar{L}_2}(\boldsymbol{e}_2)\big]_{\bar{L}}\big[Y_{\bar{L}_3}(\boldsymbol{e}_3)Y_{\bar{L}_4}(\boldsymbol{e}_4)\big]_{\bar{L}}\Big]_{00}$$
$$\Rightarrow \sum_{LL'} Z_1(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';i)\Big[\big[Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)\big]_L\big[Y_{L_3}(\boldsymbol{e}_3)Y_{L_4}(\boldsymbol{e}_4)\big]_{L'}\Big]_{\kappa\mu}, \tag{B.44}$$

and

$$[Y_1(\boldsymbol{e}_k)Y_1(\boldsymbol{e}_l)]_{\kappa\mu}\Big[\big[Y_{\bar{L}_1}(\boldsymbol{e}_1)Y_{\bar{L}_2}(\boldsymbol{e}_2)\big]_{\bar{L}}\big[Y_{\bar{L}_3}(\boldsymbol{e}_3)Y_{\bar{L}_4}(\boldsymbol{e}_4)\big]_{\bar{L}}\Big]_{00}$$
$$\Rightarrow \sum_{LL'} Z_2(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';kl)\Big[\big[Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)\big]_L\big[Y_{L_3}(\boldsymbol{e}_3)Y_{L_4}(\boldsymbol{e}_4)\big]_{L'}\Big]_{\kappa\mu}. \tag{B.45}$$

The Z_1 coefficients are given by

$$Z_1(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';1) = \delta_{\bar{L}L'}(-1)^{\kappa+\bar{L}-L}\sqrt{\frac{2L+1}{(2\kappa+1)(2\bar{L}+1)}}W(\kappa\bar{L}_1\bar{L}_2\bar{L}L),$$

$$Z_1(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';2) = \delta_{\bar{L}L'}\sqrt{\frac{2L+1}{(2\kappa+1)(2\bar{L}+1)}}W(\kappa\bar{L}_2\bar{L}_1\bar{L}L),$$

$$Z_1(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';3) = \delta_{\bar{L}L}\sqrt{\frac{2L'+1}{(2\kappa+1)(2\bar{L}+1)}}W(\kappa\bar{L}_3\bar{L}_4\bar{L}L'),$$

$$Z_1(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';4) = \delta_{\bar{L}L}(-1)^{\kappa+\bar{L}-L'}\sqrt{\frac{2L'+1}{(2\kappa+1)(2\bar{L}+1)}}W(\kappa\bar{L}_4\bar{L}_3\bar{L}L') \tag{B.46}$$

with

$$W(\kappa abcd) = C(\kappa a; \kappa + a)U(\kappa adb; \kappa + a\, c). \tag{B.47}$$

The Z_2 coefficients are given by

$$Z_2(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';12)$$
$$= \delta_{\bar{L}L'}(-1)^{\kappa+\bar{L}-L}\sqrt{\frac{2L+1}{(2\kappa+1)(2\bar{L}+1)}}C(1\bar{L}_1;L_1)C(1\bar{L}_2;L_2)\begin{bmatrix} 1 & 1 & \kappa \\ \bar{L}_1 & \bar{L}_2 & \bar{L} \\ L_1 & L_2 & L \end{bmatrix},$$

$$Z_2(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';13) = W(1\bar{L}_1\bar{L}_2\bar{L}L)W(1\bar{L}_3\bar{L}_4\bar{L}L')\begin{bmatrix} 1 & 1 & \kappa \\ \bar{L} & \bar{L} & 0 \\ L & L' & \kappa \end{bmatrix},$$

$$Z_2(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';14) = (-1)^{\bar{L}-L'+1}W(1\bar{L}_1\bar{L}_2\bar{L}L)W(1\bar{L}_4\bar{L}_3\bar{L}L')\begin{bmatrix} 1 & 1 & \kappa \\ \bar{L} & \bar{L} & 0 \\ L & L' & \kappa \end{bmatrix},$$

$$Z_2(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';23) = (-1)^{\bar{L}-L+1}W(1\bar{L}_2\bar{L}_1\bar{L}L)W(1\bar{L}_3\bar{L}_4\bar{L}L')\begin{bmatrix} 1 & 1 & \kappa \\ \bar{L} & \bar{L} & 0 \\ L & L' & \kappa \end{bmatrix},$$

$$Z_2(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';24) = (-1)^{L+L'}W(1\bar{L}_2\bar{L}_1\bar{L}L)W(1\bar{L}_4\bar{L}_3\bar{L}L')\begin{bmatrix} 1 & 1 & \kappa \\ \bar{L} & \bar{L} & 0 \\ L & L' & \kappa \end{bmatrix},$$

$$Z_2(\kappa\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL';34)$$
$$= \delta_{\bar{L}L}\sqrt{\frac{2L'+1}{(2\kappa+1)(2\bar{L}+1)}}C(1\bar{L}_3;L_3)C(1\bar{L}_4;L_4)\begin{bmatrix} 1 & 1 & \kappa \\ \bar{L}_3 & \bar{L}_4 & \bar{L} \\ L_3 & L_4 & L' \end{bmatrix}. \tag{B.48}$$

The tensor matrix element of the Gaussian radial form reads

$$\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\} Y_{2m}(\widehat{\widetilde{w}\boldsymbol{x}})|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \frac{(-1)^{L_1+L_2+L+L'}\sqrt{5}}{\sqrt{2L'+1}}\langle LM2m|L'M'\rangle \frac{c}{2}\int_0^{\frac{c}{c+c'}} du\, u^{\frac{3}{2}}$$

$$\times \left\{ \sum_{k=1}^{4}\gamma_k^2 (-1)^{\bar{L}_1+\bar{L}_2}\left(\prod_{i=1}^{4}\frac{B_{L_i}}{B_{\bar{L}_i}}\right)\sum_{\bar{L}}\sqrt{2\bar{L}+1}Z_1(2\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL'; k)\right.$$

$$\times \langle F_{(\bar{L}_3\bar{L}_4)\bar{L}\bar{M}}(u_3, u_4, A', \boldsymbol{x})|F_{(\bar{L}_1\bar{L}_2)\bar{L}\bar{M}}(u_1, u_2, A, \boldsymbol{x})\rangle\Big|_{\rho_{ij}\to\bar{\rho}_{ij}+cu\gamma_i\gamma_j}$$

$$+\sqrt{\frac{40\pi}{3}}\sum_{l>k=1}^{4}\gamma_k\gamma_l(-1)^{\bar{L}_1+\bar{L}_2}\left(\prod_{i=1}^{4}\frac{B_{L_i}}{B_{\bar{L}_i}}\right)\sum_{\bar{L}}\sqrt{2\bar{L}+1}Z_2(2\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL'; kl)$$

$$\left.\times \langle F_{(\bar{L}_3\bar{L}_4)\bar{L}\bar{M}}(u_3, u_4, A', \boldsymbol{x})|F_{(\bar{L}_1\bar{L}_2)\bar{L}\bar{M}}(u_1, u_2, A, \boldsymbol{x})\rangle\Big|_{\rho_{ij}\to\bar{\rho}_{ij}+cu\gamma_i\gamma_j}\right\}. \qquad (B.49)$$

It should be noted here that $\bar{L}_i = L_i - 2\delta_{ik}$ in the first sum of the curly bracket, whereas $\bar{L}_i = L_i - \delta_{ik} - \delta_{il}$ in the second sum. The integral appearing in Eq. (B.49) can be reduced to

$$\int_0^{\frac{c}{c+c'}} du\, u^{\frac{3}{2}}\, f(u) = 2\left(\frac{c}{c+c'}\right)^{\frac{5}{2}}\int_0^1 dx\, x^4\, f\left(\frac{c}{c+c'}x^2\right), \qquad (B.50)$$

where $f(u)$ is a polynomial function of u whose degree is at most $(\bar{L}_1+\bar{L}_2+\bar{L}_3+\bar{L}_4)/2$. This integral can therefore be accurately evaluated using the Gauss quadrature.

We note that the calculation of the tensor matrix element of the following radial form

$$\langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\} \mathcal{Y}_{2m}(\widetilde{w}\boldsymbol{x})|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle \qquad (B.51)$$

is easier. In this case the integration of Eq. (B.40) is not needed, and the above matrix element (B.51) is obtained simply by replacing u with $c/(c+c')$ in Eq. (B.49).

(iii) Spin-orbit potential

Using Eq. (B.29), we obtain

$$\langle g(\lambda_3\boldsymbol{e}_3 u_3 + \lambda_4\boldsymbol{e}_4 u_4; A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\} (\widetilde{w}\boldsymbol{x}\times\widetilde{\xi}\boldsymbol{\pi})_m|g(\lambda_1\boldsymbol{e}_1 u_1 + \lambda_2\boldsymbol{e}_2 u_2; A, \boldsymbol{x})\rangle$$

$$\longrightarrow \left(\frac{c}{c+c'}\right)^{\frac{5}{2}}\left(\frac{(2\pi)^{N-1}}{\det B}\right)^{\frac{3}{2}}\sum_{l>k=1}^{4}(\gamma_k\tau_l - \gamma_l\tau_k)\lambda_k\lambda_l\frac{\hbar}{i}(\boldsymbol{e}_k\times\boldsymbol{e}_l)_m$$

$$\times \exp\left(\sum_{j>i=1}^{4}\left[\rho_{ij} - \frac{cc'}{c+c'}\gamma_i\gamma_j\right]\lambda_i\lambda_j\boldsymbol{e}_i\cdot\boldsymbol{e}_j\right) \qquad (B.52)$$

with

$$\tau_i = \widetilde{\xi}A_i B^{-1}u_i. \qquad (B.53)$$

The difference in the matrix elements between the overlap (B.1) and the above spin-orbit potential is that the latter contains an extra factor $-i(\boldsymbol{e}_k\times\boldsymbol{e}_l)_m$.

Following the procedure similar to the one described in Eqs. (B.42), (B.43) and (B.45), we obtain the spin-orbit matrix element for the Gaussian radial form as follows:

$$\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\} (\widetilde{w}\boldsymbol{x}\times\widetilde{\xi}\boldsymbol{\pi})_m|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \frac{(-1)^{L_1+L_2+L+L'}}{\sqrt{2L'+1}}\langle LM1m|L'M'\rangle\left(4\pi\sqrt{\frac{2}{3}}\hbar\right)\left(\frac{c}{c+c'}\right)^{\frac{5}{2}}$$

$$\times \sum_{l>k=1}^{4}(\gamma_k\tau_l - \gamma_l\tau_k)(-1)^{\bar{L}_1+\bar{L}_2}\left(\prod_{i=1}^{4}\frac{B_{L_i}}{B_{\bar{L}_i}}\right)\sum_{\bar{L}}\sqrt{2\bar{L}+1}Z_2(1\bar{L}_1\bar{L}_2\bar{L}_3\bar{L}_4\bar{L}, LL'; kl)$$

$$\times \langle F_{(\bar{L}_3\bar{L}_4)\bar{L}\bar{M}}(u_3, u_4, A', \boldsymbol{x})|F_{(\bar{L}_1\bar{L}_2)\bar{L}\bar{M}}(u_1, u_2, A, \boldsymbol{x})\rangle\Big|_{\rho_{ij}\to\rho_{ij}-\frac{cc'}{c+c'}\gamma_i\gamma_j}, \qquad (B.54)$$

where $\bar{L}_i$ is defined by $L_i - \delta_{ik} - \delta_{il}$ depending on the summation labels k and l.

<u>(iv) Multipole moment</u>

We calculate the matrix element for a multipole moment operator. Using Eqs. (B.18) and (B.20) with $V(\boldsymbol{r}) = \mathcal{Y}_{\ell m}(\boldsymbol{r})$, we obtain

$$
\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) | \mathcal{Y}_{\ell m}(\widetilde{w}\boldsymbol{x}) | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle
$$
$$
\longrightarrow \int d\boldsymbol{r}\, \mathcal{Y}_{\ell m}(\boldsymbol{r}) \left(\frac{(2\pi)^{N-2} c}{\det B} \right)^{\frac{3}{2}} \exp \left(-\frac{1}{2} c r^2 + \sum_{j>i=1}^{4} \bar{\rho}_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j + c \sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i \cdot \boldsymbol{r} \right)
$$
$$
= \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \mathcal{Y}_{\ell m} \left(\sum_{i=1}^{4} \gamma_i \lambda_i \boldsymbol{e}_i \right) \exp \left(\sum_{j>i=1}^{4} \rho_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right). \tag{B.55}
$$

In the case of $\ell = 2$, the above result is compared to Eq. (B.41). That is, it is simply obtained by dropping $c/2$ and by setting $u = 1$. Therefore the matrix element

$$
\langle F_{(L_3 L_4) LM}(u_3, u_4, A', \boldsymbol{x}) | \mathcal{Y}_{2m}(\widetilde{w}\boldsymbol{x}) | F_{(L_1 L_2) LM}(u_1, u_2, A, \boldsymbol{x}) \rangle
$$

is obtained from Eq. (B.49) by the same procedure as noted above.

It is easy to obtain the matrix element for the dipole operator ($\ell = 1$) in a similar way:

$$
\langle F_{(L_3 L_4) L'M'}(u_3, u_4, A', \boldsymbol{x}) | \mathcal{Y}_{1m}(\widetilde{w}\boldsymbol{x}) | F_{(L_1 L_2) LM}(u_1, u_2, A, \boldsymbol{x}) \rangle
$$
$$
= \frac{(-1)^{L_1 + L_2 + L + L' + 1} \sqrt{3}}{\sqrt{2L'+1}} \langle LM1m | L'M' \rangle
$$
$$
\times \sum_{k=1}^{4} \gamma_k (-1)^{\bar{L}_1 + \bar{L}_2} \left(\prod_{i=1}^{4} \frac{B_{L_i}}{B_{\bar{L}_i}} \right) \sum_{\bar{L}} \sqrt{2\bar{L}+1}\, Z_1(1\bar{L}_1 \bar{L}_2 \bar{L}_3 \bar{L}_4 \bar{L}, LL'; k)
$$
$$
\times \langle F_{(\bar{L}_3 \bar{L}_4) \bar{L} \bar{M}}(u_3, u_4, A', \boldsymbol{x}) | F_{(\bar{L}_1 \bar{L}_2) \bar{L} \bar{M}}(u_1, u_2, A, \boldsymbol{x}) \rangle, \tag{B.56}
$$

where $\bar{L}_i$ is defined by $\bar{L}_i = L_i - \delta_{ik}$ depending on the summation label k.

B.5 Many-particle correlation function

A many-particle correlation function is useful to visualize the structure of a system [6, 21, 40, 41, 26]. The function is defined by the matrix element of the product of n δ-functions ($n \leq N-1$), e.g., $\delta(\boldsymbol{r}_i - \boldsymbol{r}_j - \boldsymbol{d}_1) \delta(\boldsymbol{r}_k - \boldsymbol{r}_l - \boldsymbol{d}_2) \cdots = \delta(\widetilde{w^{(1)}}\boldsymbol{x} - \boldsymbol{d}_1) \delta(\widetilde{w^{(2)}}\boldsymbol{x} - \boldsymbol{d}_2) \cdots$. The basic matrix element is the one between the generating functions:

$$
\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) | \prod_{\alpha=1}^{n} \delta(\widetilde{w^{(\alpha)}}\boldsymbol{x} - \boldsymbol{d}_\alpha) | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle
$$
$$
= \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \left(\frac{\det \mathcal{C}}{(2\pi)^n} \right)^{\frac{3}{2}} \exp \left(\frac{1}{2} \widetilde{\boldsymbol{v}} B^{-1} \boldsymbol{v} - \frac{1}{2} \boldsymbol{Q} \mathcal{C} \boldsymbol{Q} \right), \tag{B.57}
$$

which is obtained by expressing the δ-functions as Fourier integrals, and where

$$
(\mathcal{C}^{-1})_{\alpha\beta} = \widetilde{w^{(\alpha)}} B^{-1} w^{(\beta)}, \qquad \boldsymbol{Q}_\alpha = \widetilde{w^{(\alpha)}} B^{-1} \boldsymbol{v} - \boldsymbol{d}_\alpha, \qquad (\alpha, \beta = 1, ..., n). \tag{B.58}
$$

Omitting the λ_i^2 terms leads to

$$
\frac{1}{2} \widetilde{\boldsymbol{v}} B^{-1} \boldsymbol{v} - \frac{1}{2} \boldsymbol{Q} \mathcal{C} \boldsymbol{Q} \longrightarrow \sum_{j>i=1}^{4} \bar{\varrho}_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j + \sum_{i=1}^{4} \lambda_i \boldsymbol{e}_i \cdot \boldsymbol{D}_i - \frac{1}{2} \widetilde{\boldsymbol{d}} \mathcal{C} \boldsymbol{d}, \tag{B.59}
$$

where $\boldsymbol{d}$ is a one-column matrix consisting of $\boldsymbol{d}_1, ..., \boldsymbol{d}_n$, and

$$
\bar{\varrho}_{ij} = \rho_{ij} - (\widetilde{\Gamma} \mathcal{C} \Gamma)_{ij}, \qquad \boldsymbol{D}_i = (\widetilde{\Gamma} \mathcal{C} \boldsymbol{d})_i \tag{B.60}
$$

with

$$
\Gamma_{\alpha i} = \widetilde{w^{(\alpha)}} B^{-1} u_i, \qquad (\alpha = 1, ..., n;\ i = 1, ..., 4). \tag{B.61}
$$

Following the same procedure as in Appendix B.3 (cf. Eq. (B.23)) leads to

$$\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x})| \prod_{\alpha=1}^{n} \delta(\widetilde{w^{(\alpha)}}\boldsymbol{x} - \boldsymbol{d}_\alpha)|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \frac{(-1)^{L_1+L_2+L+M+L'+M'}}{\sqrt{2L'+1}} \left(\prod_{i=1}^{4} B_{L_i}\right) \left(\frac{(2\pi)^{N-1}}{\det B}\right)^{\frac{3}{2}} \left(\frac{\det \mathcal{C}}{(2\pi)^n}\right)^{\frac{3}{2}} \exp\left(-\frac{1}{2}\widetilde{\boldsymbol{d}}\mathcal{C}\boldsymbol{d}\right)$$

$$\times \sum_{p_{ij}} \left(\prod_{j>i=1}^{4} \frac{(-1)^{p_{ij}}\sqrt{2p_{ij}+1}}{B_{p_{ij}}}(\bar{\varrho}_{ij})^{p_{ij}}\right) \sum_{q_i} \left(\prod_{i=1}^{4} \frac{(-1)^{q_i}}{B_{q_i}}\right)$$

$$\times \sum_{\kappa\mu\mu'\ell m} \langle LM\ell m|L'M'\rangle\sqrt{2\ell+1}X(p_{13}p_{14}p_{23}p_{24};\kappa)$$

$$\times Y(p_{12}p_{12}p_{34}p_{34}\ p_{13}+p_{14}\ p_{23}+p_{24}\ p_{13}+p_{23}\ p_{14}+p_{24}\ 0\kappa\kappa0;\kappa\kappa)$$

$$\times Y(L_1-q_1\ L_2-q_2\ L_3-q_3\ L_4-q_4\ q_1q_2q_3q_4\kappa\mu\mu'\ell;LL')$$

$$\times [[\mathcal{Y}_{q_1}(\boldsymbol{D}_1)\mathcal{Y}_{q_2}(\boldsymbol{D}_2)]_\mu[\mathcal{Y}_{q_3}(\boldsymbol{D}_3)\mathcal{Y}_{q_4}(\boldsymbol{D}_4)]_{\mu'}]_{\ell-m}. \tag{B.62}$$

The values of p_{ij} and q_i are restricted by the condition of Eq. (B.24).

Note that the matrix element of a many-body force is readily evaluated using Eq (B.62).

Appendix C: Integral transform of the correlated Gaussian basis

C.1 Integral transform of the generating function

An integral transform of the CG is needed to adapt nonlocal RGM kernels into a variational calculation. A typical form of the kernel we consider is

$$K(\boldsymbol{r}', \boldsymbol{r}) = \exp\left(-\frac{1}{2}p'\boldsymbol{r}'^2 - \frac{1}{2}p\boldsymbol{r}^2 - q\boldsymbol{r}' \cdot \boldsymbol{r}\right), \tag{C.1}$$

where $\boldsymbol{r}$ is one of the relative distance vectors, say, between particles k and l. Thus $\boldsymbol{r}$ denotes $\widetilde{w}\boldsymbol{x}$ (see Eq. (4.1)). The vector $\boldsymbol{r}'$ is defined in exactly the same way as $\boldsymbol{r}$.

In order to calculate the integral transform acted by K on the basis function (2.7), we start from its action on the generating function

$$[Kg](\boldsymbol{x}) = \int d\boldsymbol{r}\, K(\boldsymbol{r}', \boldsymbol{r})g(\boldsymbol{s}; A, \boldsymbol{x}). \tag{C.2}$$

The operator K acting on the function g changes it to a new function Kg, which is again a function of $\boldsymbol{x}$ because $\boldsymbol{r}'$ denotes $\widetilde{w}\boldsymbol{x}$.

The first step of obtaining $[Kg](\boldsymbol{x})$ is to transform the coordinate set $\boldsymbol{x}$ to a set of coordinates $\boldsymbol{y} = \{\boldsymbol{y}_1, ..., \boldsymbol{y}_{N-1}\}$:

$$\boldsymbol{y}_i = \sum_{k=1}^{N-1} (w^{(i)})_k \boldsymbol{x}_k = \widetilde{w^{(i)}}\boldsymbol{x}, \qquad w^{(1)} = w. \tag{C.3}$$

The vector $w^{(i)}$ is chosen in such a way that the first coordinate $\boldsymbol{y}_1$ reduces to $\widetilde{w}\boldsymbol{x} = \boldsymbol{r}_k - \boldsymbol{r}_l$. The choice of other relative coordinates $\{\boldsymbol{y}_2, ..., \boldsymbol{y}_{N-1}\}$, namely $w^{(i)}$ $(i = 2, ..., N-1)$, is not unique. Their choice is, however, subject to the condition that any of $\{\boldsymbol{y}_2, ..., \boldsymbol{y}_{N-1}\}$ must be independent of $\boldsymbol{y}_1$, that is, it may contain $\boldsymbol{r}_k$ and $\boldsymbol{r}_l$ only as a combination of $(m_k\boldsymbol{r}_k+m_l\boldsymbol{r}_l)/(m_k+m_l)$ but not as $\boldsymbol{r}_k$ or $\boldsymbol{r}_l$ alone; otherwise the integration over $\boldsymbol{r} = \boldsymbol{r}_k - \boldsymbol{r}_l$ in Eq. (C.2) cannot be performed as it is meant. The coordinate transformation (C.3) from $\boldsymbol{x}$ to $\boldsymbol{y}$ is expressed as $\boldsymbol{y} = T^{-1}\boldsymbol{x}$ by the matrix T^{-1}:

$$T^{-1} = \begin{pmatrix} \widetilde{w^{(1)}} \\ \widetilde{w^{(2)}} \\ \vdots \\ \widetilde{w^{(N-1)}} \end{pmatrix}. \tag{C.4}$$

The transformation from $\boldsymbol{y}$ to $\boldsymbol{x}$, $\boldsymbol{x} = T\boldsymbol{y}$, reads as

$$T = \left(\zeta^{(1)} \ \zeta^{(2)} \cdots \zeta^{(N-1)} \right), \qquad \zeta^{(1)} = \zeta. \tag{C.5}$$

Since $T^{-1}T = TT^{-1} = 1$, we have

$$\widetilde{w^{(i)}}\zeta^{(j)} = \widetilde{\zeta^{(i)}}w^{(j)} = \delta_{ij}, \qquad \sum_{k=1}^{N-1} \zeta_i^{(k)} w_j^{(k)} = \delta_{ij}. \tag{C.6}$$

The second equation is rewritten in a matrix form as

$$\sum_{k=2}^{N-1} \zeta^{(k)}\widetilde{w^{(k)}} = 1 - \zeta\widetilde{w}, \quad \text{or} \quad \sum_{k=2}^{N-1} w^{(k)}\widetilde{\zeta^{(k)}} = 1 - w\widetilde{\zeta}. \tag{C.7}$$

The next step is to substitute $\boldsymbol{x} = T\boldsymbol{y}$ to g and to separate the part depending on $\boldsymbol{y}_1$:

$$
\begin{aligned}
g(\boldsymbol{s}; A, \boldsymbol{x}) &= g(\widetilde{T}\boldsymbol{s}; \widetilde{T}AT, \boldsymbol{y}) \\
&= \exp\left(-\frac{1}{2}a\boldsymbol{y}_1^2 + \boldsymbol{t}\cdot\boldsymbol{y}_1 - \widetilde{a^{(1)}}\boldsymbol{y}^{(1)} \cdot \boldsymbol{y}_1 \right) g(\boldsymbol{t}^{(1)}; A^{(1)}, \boldsymbol{y}^{(1)}),
\end{aligned}
\tag{C.8}
$$

where we introduce short-hand notations for the matrix $\widetilde{T}AT$ and the vectors, $\widetilde{T}\boldsymbol{s}$ and $\boldsymbol{y}$, by

$$\widetilde{T}AT = \begin{pmatrix} a & \widetilde{a^{(1)}} \\ a^{(1)} & A^{(1)} \end{pmatrix}, \qquad \widetilde{T}\boldsymbol{s} = \begin{pmatrix} \boldsymbol{t} \\ \boldsymbol{t}^{(1)} \end{pmatrix}, \qquad \boldsymbol{y} = \begin{pmatrix} \boldsymbol{y}_1 \\ \boldsymbol{y}^{(1)} \end{pmatrix}. \tag{C.9}$$

Here $a^{(1)}$ is an $(N-2)$-dimensional column vector, $A^{(1)}$ an $(N-2)\times(N-2)$ symmetric matrix, and $\boldsymbol{t}^{(1)}$ is an $(N-2)$-dimensional column vector whose element is a 3-dimensional vector. More explicitly they are given by

$$
\begin{aligned}
a &= \widetilde{\zeta}A\zeta, & a_i^{(1)} &= \widetilde{\zeta^{(i+1)}}A\zeta, & A_{ij}^{(1)} &= \widetilde{\zeta^{(i+1)}}A\zeta^{(j+1)}, \\
\boldsymbol{t} &= \widetilde{\zeta}\boldsymbol{s}, & \boldsymbol{t}_i^{(1)} &= \widetilde{\zeta^{(i+1)}}\boldsymbol{s},
\end{aligned}
\tag{C.10}
$$

where $i, j = 1, 2, \ldots, N-2$. Substituting Eqs. (C.8) and (C.1) into Eq. (C.2), integrating over $\boldsymbol{r} = \boldsymbol{y}_1$ and then renaming $\boldsymbol{r}' = \boldsymbol{y}_1$ lead to

$$[Kg](\boldsymbol{x}) = \left(\frac{2\pi}{a+p}\right)^{\frac{3}{2}} \exp\left(\frac{1}{2(a+p)}\boldsymbol{t}^2\right) g(\bar{\boldsymbol{s}}; \bar{A}, \boldsymbol{y}), \tag{C.11}$$

where

$$\bar{A} = \begin{pmatrix} p' - \frac{q^2}{a+p} & -\frac{q}{a+p}\widetilde{a^{(1)}} \\ -\frac{q}{a+p}a^{(1)} & A^{(1)} - \frac{1}{a+p}a^{(1)}\widetilde{a^{(1)}} \end{pmatrix}, \qquad \bar{\boldsymbol{s}} = \begin{pmatrix} -\frac{q}{a+p}\boldsymbol{t} \\ \boldsymbol{t}^{(1)} - \frac{1}{a+p}\boldsymbol{t}a^{(1)} \end{pmatrix}. \tag{C.12}$$

The last step is to express the above function $g(\bar{\boldsymbol{s}}; \bar{A}, \boldsymbol{y})$ in terms of $\boldsymbol{x}$. This is achieved by replacing $\boldsymbol{y}$ with $T^{-1}\boldsymbol{x}$ (see Eqs. (2.11) and (2.12)):

$$g(\bar{\boldsymbol{s}}; \bar{A}, \boldsymbol{y}) = g(\widetilde{T^{-1}}\bar{\boldsymbol{s}}; \widetilde{T^{-1}}\bar{A}T^{-1}, \boldsymbol{x}) = g(Q_K\boldsymbol{s}; A_K, \boldsymbol{x}), \tag{C.13}$$

where the matrices Q_K and A_K turn out to be given by

$$Q_K = 1 - \frac{p+q}{a+p}w\widetilde{\zeta} - \frac{1}{a+p}A\zeta\widetilde{\zeta},$$

$$A_K = A + \left(a + p' - \frac{(a-q)^2}{a+p}\right)w\widetilde{w} - \frac{p+q}{a+p}\left(w\widetilde{\zeta}A + A\zeta\widetilde{w}\right) - \frac{1}{a+p}A\zeta\widetilde{\zeta}A. \tag{C.14}$$

Substitution of Eqs. (C.10) and (C.13) in Eq. (C.11) leads to the desired result

$$[Kg](\boldsymbol{x}) = \left(\frac{2\pi}{a+p}\right)^{\frac{3}{2}} \exp\left(\frac{1}{2(a+p)}\widetilde{\boldsymbol{s}}\zeta\widetilde{\zeta}\boldsymbol{s}\right) g(Q_K\boldsymbol{s}; A_K, \boldsymbol{x}). \tag{C.15}$$

Using this result (C.15) with $s = \lambda_1 e_1 u_1 + \lambda_2 e_2 u_2$ in Eq. (2.9), we can derive

$$[KF_{(L_1 L_2)LM}(u_1, u_2, A)](\boldsymbol{x}) = \left(\frac{2\pi}{a+p}\right)^{\frac{3}{2}} \sum_{\ell=0}^{\ell_M} \mathcal{K}(L_1 L_2 L; \ell) \left(\frac{\widetilde{u_1}\zeta\widetilde{\zeta}u_2}{a+p}\right)^\ell$$
$$\times F_{(L_1-\ell\, L_2-\ell)LM}(Q_K u_1, Q_K u_2, A_K, \boldsymbol{x}), \qquad \text{(C.16)}$$

where $\ell_M = \min(L_1, L_2, [(L_1 + L_2 - L)/2])$ and $\mathcal{K}(L_1 L_2 L; \ell)$ is defined in Eq. (A.8). The action of the integral kernel on the CG with two GV leads to that of the same kinds. In particular we obtain a very simple result for the CG of types of Eqs. (2.4) and (2.6):

$$[KF_{(L0)LM}(u_1, u_2, A)](\boldsymbol{x}) = \left(\frac{2\pi}{a+p}\right)^{\frac{3}{2}} F_{(L0)LM}(Q_K u_1, Q_K u_2, A_K, \boldsymbol{x}),$$

$$[KF_{(L1)LM}(u_1, u_2, A)](\boldsymbol{x}) = \left(\frac{2\pi}{a+p}\right)^{\frac{3}{2}} F_{(L1)LM}(Q_K u_1, Q_K u_2, A_K, \boldsymbol{x}). \qquad \text{(C.17)}$$

Apparently both $[Kg](\boldsymbol{x})$ and $[KF_{(L_1 L_2)LM}(u_1, u_2, A)](\boldsymbol{x})$ should not depend on the choice of $w^{(i)}$ $(i = 2, \ldots, N-1)$. This is equivalent to the statement that both Q_K and A_K are independent of the choice of $w^{(i)}$ $(i = 2, \ldots, N-1)$. For this to hold true, it is sufficient to show that ζ is independent of that choice. In order to prove this, let $w'^{(i)}$ $(i = 2, \ldots, N-1)$ denote a set of other choice. They are related to the original set $w^{(i)}$ $(i = 2, \ldots, N-1)$ by a non-singular linear transformation W as

$$\left(w'^{(2)} \cdots w'^{(N-1)}\right) = \left(w^{(2)} \cdots w^{(N-1)}\right) W. \qquad \text{(C.18)}$$

The coordinate transformation from $\boldsymbol{x}$ to $\boldsymbol{y}'$ $(\boldsymbol{y}'_i = \widetilde{w'^{(i)}}\boldsymbol{x})$ is performed by a matrix T'^{-1}:

$$T'^{-1} = \begin{pmatrix} \widetilde{w} \\ \widetilde{w'^{(2)}} \\ \vdots \\ \widetilde{w'^{(N-1)}} \end{pmatrix}. \qquad \text{(C.19)}$$

Using Eqs. (C.4), (C.18) and (C.19) enables one to show $T'^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & \widetilde{W} \end{pmatrix} T^{-1}$, leading to

$$T' = T \begin{pmatrix} 1 & 0 \\ 0 & \widetilde{W}^{-1} \end{pmatrix}. \qquad \text{(C.20)}$$

This equation indicates that the first column of the matrix T' is the same as that of T, namely ζ, so that ζ remains the same against any choice of W.

C.2 Determination of ζ

The vector ζ is determined by the condition $\widetilde{w^{(i)}}\zeta = \delta_{i1}$. See Eq. (C.6). As shown below, it is possible to determine ζ without specifying $w^{(i)}$ $(i = 2, \ldots, N-1)$.

Any of $\{\boldsymbol{y}_2, \ldots, \boldsymbol{y}_{N-1}\}$ is expressed as a linear combination of $\boldsymbol{r}_i$ as

$$\sum_{i=1}^N a_i \boldsymbol{r}_i, \qquad \text{(C.21)}$$

where a_i may be taken arbitrarily provided that they satisfy the following conditions

$$a_k = \frac{m_k}{m_k + m_l}\lambda, \qquad a_l = \frac{m_l}{m_k + m_l}\lambda, \qquad \sum_{i=1}^N a_i = 0. \qquad \text{(C.22)}$$

The last equation assures that $\boldsymbol{y}_i$, as one of the relative coordinates, has no dependence on the center of mass coordinate. The λ value is determined as

$$\lambda = -\sum_{i \neq k, l} a_i. \qquad \text{(C.23)}$$

Substitution of $\boldsymbol{r}_i = \sum_{j=1}^{N}(U^{-1})_{ij}\boldsymbol{x}_j$ (see Eq. (2.3)) enables one to express the vector (C.21) in terms of the coordinate $\boldsymbol{x}$ as

$$\sum_{i=1}^{N} a_i \boldsymbol{r}_i = \sum_{j=1}^{N} (\widetilde{U^{-1}a})_j \boldsymbol{x}_j, \tag{C.24}$$

which indicates that the j-th element of $w^{(i)}$ is given by $(\widetilde{U^{-1}a})_j$. The condition to determine ζ is thus expressed as

$$\sum_{j=1}^{N-1} w_j \zeta_j = \sum_{j=1}^{N-1} \left[(U^{-1})_{kj} - (U^{-1})_{lj} \right] \zeta_j = 1, \qquad \sum_{j=1}^{N-1} (\widetilde{U^{-1}a})_j \zeta_j = 0. \tag{C.25}$$

Using Eqs. (C.22) and (C.23) reduces the second equation in Eq. (C.25) to

$$\sum_{i=1}^{N} \sum_{j=1}^{N-1} (U^{-1})_{ij} \zeta_j a_i = \sum_{i \neq k,l} (U^{-1}\zeta)_i a_i + (U^{-1}\zeta)_k a_k + (U^{-1}\zeta)_l a_l$$

$$= \sum_{i \neq k,l} \left[(U^{-1}\zeta)_i - \frac{m_k}{m_k+m_l}(U^{-1}\zeta)_k - \frac{m_l}{m_k+m_l}(U^{-1}\zeta)_l \right] a_i = 0. \tag{C.26}$$

Since a_i $(i \neq k, l)$ can be taken arbitrarily, the coefficients of a_i must vanish, that is,

$$\sum_{j=1}^{N-1} \left[(U^{-1})_{ij} - \frac{m_k}{m_k+m_l}(U^{-1})_{kj} - \frac{m_l}{m_k+m_l}(U^{-1})_{lj} \right] \zeta_j = 0 \qquad \text{for } i \neq k,l. \tag{C.27}$$

The solution of the first equation in Eq. (C.25) together with the above equation determines ζ.

C.3 ℓ^2-dependent potential of Gaussian radial form

As a useful application of the decomposition of Eq. (C.8), we calculate the matrix element of an ℓ^2-dependent potential of Gaussian radial form, where the angular momentum $\boldsymbol{\ell}$ is defined as $\boldsymbol{\ell} = \boldsymbol{y}_1 \times (-i\hbar)\partial/\partial \boldsymbol{y}_1$ with $\boldsymbol{y}_1 = \widetilde{w}\boldsymbol{x} = \boldsymbol{r}_k - \boldsymbol{r}_l$. Using Eq. (C.8) we obtain

$$\boldsymbol{\ell}\, g(\boldsymbol{s}; A, \boldsymbol{x}) = \frac{\hbar}{i} \widetilde{w}\boldsymbol{x} \times \left(\boldsymbol{t} - \widetilde{a^{(1)}}\boldsymbol{y}^{(1)} \right) g(\boldsymbol{s}; A, \boldsymbol{x}) = \frac{\hbar}{i} \widetilde{w}\boldsymbol{x} \times (\widetilde{\zeta}\boldsymbol{s} - \widetilde{\zeta}A\boldsymbol{x})\, g(\boldsymbol{s}; A, \boldsymbol{x}), \tag{C.28}$$

where use is made of $\boldsymbol{t} = \widetilde{\zeta}\boldsymbol{s}$ and $\widetilde{a^{(1)}}\boldsymbol{y}^{(1)} = \widetilde{\zeta}A\boldsymbol{x} - a\widetilde{w}\boldsymbol{x}$ in the last step.

Using the property of $\boldsymbol{\ell}^2 = \boldsymbol{\ell} \cdot \boldsymbol{\ell} = \boldsymbol{\ell}^\dagger \cdot \boldsymbol{\ell}$ and the fact that $\boldsymbol{\ell}$ commutes with a scalar function leads to an expression for the matrix element between the generating functions as follows:

$$\langle g(\boldsymbol{s}'; A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\} \boldsymbol{\ell}^2 | g(\boldsymbol{s}; A, \boldsymbol{x}) \rangle$$

$$= \hbar^2 \langle g(\boldsymbol{s}'; A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\} \mathcal{L}^2 | g(\boldsymbol{s}; A, \boldsymbol{x}) \rangle \tag{C.29}$$

with

$$\begin{aligned}
\mathcal{L}^2 &= \left(\widetilde{w}\boldsymbol{x} \times (\widetilde{\zeta}\boldsymbol{s}' - \widetilde{\zeta}A'\boldsymbol{x}) \right) \cdot \left(\widetilde{w}\boldsymbol{x} \times (\widetilde{\zeta}\boldsymbol{s} - \widetilde{\zeta}A\boldsymbol{x}) \right) \\
&= \widetilde{\boldsymbol{x}}w\widetilde{w}\boldsymbol{x} \left(\widetilde{\boldsymbol{s}}'\zeta\widetilde{\zeta}\boldsymbol{s} - \widetilde{\boldsymbol{s}}'\zeta\widetilde{\zeta}A\boldsymbol{x} - \widetilde{\boldsymbol{s}}\zeta\widetilde{\zeta}A'\boldsymbol{x} + \widetilde{\boldsymbol{x}}A'\zeta\widetilde{\zeta}A\boldsymbol{x} \right) \\
&\quad - \left(\widetilde{\boldsymbol{s}}'\zeta\widetilde{w}\boldsymbol{x} - \widetilde{\boldsymbol{x}}A'\zeta\widetilde{w}\boldsymbol{x} \right)\left(\widetilde{\boldsymbol{s}}\zeta\widetilde{w}\boldsymbol{x} - \widetilde{\boldsymbol{x}}A\zeta\widetilde{w}\boldsymbol{x} \right). \tag{C.30}
\end{aligned}$$

The integration in Eq. (C.29) is elementary. It reduces to the following result

$$\langle\, g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\} \boldsymbol{\ell}^2 | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle$$

$$\longrightarrow \hbar^2 \left(\frac{c}{c+c'} \right)^{\frac{3}{2}} \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \exp\left(\sum_{j>i=1}^{4} \left[\rho_{ij} - \frac{cc'}{c+c'}\gamma_i\gamma_j \right] \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \right)$$

$$\times \left(L^{(0)} + 2 \sum_{j>i=1}^{4} L^{(1)}_{ij} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j + 4 \sum_{j>i=1}^{4} \sum_{l>k=1}^{4} L^{(2)}_{ij,kl} \lambda_i \lambda_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j \lambda_k \lambda_l \boldsymbol{e}_k \cdot \boldsymbol{e}_l \right). \tag{C.31}$$

Here the constants $L^{(0)}$, $L_{ij}^{(1)}$ and $L_{ij,kl}^{(2)}$ are determined through w, ζ, u_1, u_2, u_3, u_4, A, A', c'. Their expressions are lengthy and not written here. Substitution of Eq. (C.31) into Eq. (3.2) makes it possible to relate the desired matrix element to the overlap matrix element by

$$\langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})| \exp\left\{ -\frac{1}{2}c'(\widetilde{w}\boldsymbol{x})^2 \right\}\ell^2 |F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$

$$= \hbar^2 \left(\frac{c}{c+c'} \right)^{\frac{3}{2}} \left(L^{(0)} + 2\sum_{j>i=1}^{4} L_{ij}^{(1)} \frac{\partial}{\partial \rho_{ij}} + 4\sum_{j>i=1}^{4}\sum_{l>k=1}^{4} L_{ij,kl}^{(2)} \frac{\partial^2}{\partial \rho_{ij}\partial \rho_{kl}} \right)$$

$$\times \langle F_{(L_3 L_4)LM}(u_3, u_4, A', \boldsymbol{x})|F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle \Big|_{\rho_{ij}\to\rho_{ij}-\frac{cc'}{c+c'}\gamma_i\gamma_j}. \qquad \text{(C.32)}$$

Appendix D: Matrix elements of nonlocal operators

D.1 Nonlocal operator matrix element for the generating function

To prove Eq. (4.4), we start from the matrix element of the nonlocal operator (4.3) for the generating function. With use of Eq. (C.8) on the bra-ket generating functions, we obtain [21]

$$\langle g(\boldsymbol{s}'; A', \boldsymbol{x}) \mid V_{\mathrm{NL}} \mid g(\boldsymbol{s}; A, \boldsymbol{x})\rangle = \int\int d\boldsymbol{r}' d\boldsymbol{r} V(\boldsymbol{r}', \boldsymbol{r}) \exp\left(-\frac{1}{2}a'\boldsymbol{r}'^2 + \boldsymbol{t}'\cdot\boldsymbol{r}' - \frac{1}{2}a\boldsymbol{r}^2 + \boldsymbol{t}\cdot\boldsymbol{r} \right)$$

$$\times \mid \det T \mid^3 \left(\frac{(2\pi)^{N-2}}{\det(A^{(1)} + A'^{(1)})} \right)^{\frac{3}{2}} \exp\left(\frac{1}{2}\widetilde{\boldsymbol{d}}(A^{(1)} + A'^{(1)})^{-1}\boldsymbol{d} \right), \qquad \text{(D.1)}$$

where $|\det T|^3$ is the Jacobian, $\det(\partial\boldsymbol{x}/\partial\boldsymbol{y})$, for the transformation from $\boldsymbol{x}$ to $\boldsymbol{y}$, and

$$\boldsymbol{d} = \boldsymbol{t}^{(1)} - a^{(1)}\boldsymbol{r} + \boldsymbol{t}'^{(1)} - a'^{(1)}\boldsymbol{r}' = \begin{pmatrix} \widetilde{\zeta^{(2)}} \\ \widetilde{\zeta^{(3)}} \\ \vdots \\ \widetilde{\zeta^{(N-1)}} \end{pmatrix} \boldsymbol{D}, \qquad \text{(D.2)}$$

with

$$\boldsymbol{D} = \boldsymbol{s} + \boldsymbol{s}' - A\zeta\boldsymbol{r} - A'\zeta\boldsymbol{r}'. \qquad \text{(D.3)}$$

Here a', $a'^{(1)}$, $A'^{(1)}$, $\boldsymbol{t}'$, $\boldsymbol{t}'^{(1)}$ are defined in exactly the same way as the corresponding quantities given in Eq. (C.10) by replacing A and $\boldsymbol{s}$ with A' and $\boldsymbol{s}'$.

The matrix element (D.1) must be independent of the choice of $(w^{(2)}, \ldots, w^{(N-1)})$ from its construction. This is indeed assured by a theorem

$$\det(A^{(1)} + A'^{(1)}) = \frac{1}{c}(\det T)^2 \det B,$$

$$\widetilde{\boldsymbol{d}}(A^{(1)} + A'^{(1)})^{-1}\boldsymbol{d} = \widetilde{\boldsymbol{D}}J^{-1}\boldsymbol{D}, \qquad \text{(D.4)}$$

where c and J^{-1} are given in Eq. (4.5). Substituting these results in Eq. (D.1) leads to the result (4.4), which is manifestly independent of the choice of $w^{(i)}$.

D.2 Proof of a theorem (D.4)

With a slight change of notation the above theorem is stated as follows.

(Theorem) Let A be an $(N-1)\times(N-1)$ real, symmetric, positive-definite matrix and T be an $(N-1)\times(N-1)$ non-singular matrix given by Eq. (C.5). Let a matrix $\widetilde{T}AT$ be decomposed into

$$\widetilde{T}AT = \begin{pmatrix} a & \widetilde{a^{(1)}} \\ a^{(1)} & A^{(1)} \end{pmatrix}, \qquad \text{(D.5)}$$

where a, $a^{(1)}$ and $A^{(1)}$ are defined by Eq. (C.10). The theorem reads

$$\det A^{(1)} = \frac{1}{\alpha}(\det T)^2 \det A, \tag{D.6}$$

$$\left(\zeta^{(2)}\zeta^{(3)}\cdots\zeta^{(N-1)}\right)(A^{(1)})^{-1}\begin{pmatrix}\widetilde{\zeta^{(2)}}\\\widetilde{\zeta^{(3)}}\\\vdots\\\widetilde{\zeta^{(N-1)}}\end{pmatrix} = A^{-1} - \alpha A^{-1}w\widetilde{w}A^{-1}, \tag{D.7}$$

with

$$\alpha = (\widetilde{w}A^{-1}w)^{-1}, \tag{D.8}$$

and a row vector $\widetilde{w}$ is the first row of T^{-1} as defined in Eq. (C.4).

(Proof) The heart of this theorem lies in that the quantities on the left sides of Eqs. (D.6) and (D.7) are determined by w alone. The theorem was proved by one of the authors (Y.S.) [21]. We here show its proof as the application of nonlocal operators becomes increasingly important.

We can make use of the following identity

$$\begin{pmatrix} a & \widetilde{a^{(1)}} \\ a^{(1)} & A^{(1)} \end{pmatrix}\begin{pmatrix} 1 & -\frac{1}{a}\widetilde{a^{(1)}} \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} a & 0 \\ a^{(1)} & A^{(1)} - \frac{1}{a}a^{(1)}\widetilde{a^{(1)}} \end{pmatrix}, \tag{D.9}$$

because $a = \widetilde{\zeta}A\zeta$ is not zero thanks to the positive-definiteness of A. Taking the determinant of the above equation, we have

$$\det\begin{pmatrix} a & \widetilde{a^{(1)}} \\ a^{(1)} & A^{(1)} \end{pmatrix} = (\det T)^2\det A = a\det\left(A^{(1)} - \frac{1}{a}a^{(1)}\widetilde{a^{(1)}}\right). \tag{D.10}$$

Using the Sherman-Morrison formula [9, 42] reduces the right side of Eq. (D.10) to

$$a\left(1 - \frac{1}{a}\widetilde{a^{(1)}}(A^{(1)})^{-1}a^{(1)}\right)\det A^{(1)}. \tag{D.11}$$

To calculate $x = \widetilde{a^{(1)}}(A^{(1)})^{-1}a^{(1)}$, we invert Eq. (D.9), obtaining

$$\begin{pmatrix} 1 & \frac{1}{a}\widetilde{a^{(1)}} \\ 0 & 1 \end{pmatrix}T^{-1}A^{-1}\widetilde{T}^{-1} = \begin{pmatrix} \frac{1}{a} & 0 \\ -\frac{1}{a}\left(A^{(1)} - \frac{1}{a}a^{(1)}\widetilde{a^{(1)}}\right)^{-1}a^{(1)} & \left(A^{(1)} - \frac{1}{a}a^{(1)}\widetilde{a^{(1)}}\right)^{-1} \end{pmatrix}. \tag{D.12}$$

Let G denote an $(N-2)\times(N-2)$ matrix which is obtained by removing the first row and first column from the above matrix. Comparing both sides of Eq. (D.12) leads to

$$\begin{aligned} G &\equiv \begin{pmatrix}\widetilde{w^{(2)}}\\\widetilde{w^{(3)}}\\\vdots\\\widetilde{w^{(N-1)}}\end{pmatrix}A^{-1}\left(w^{(2)}w^{(3)}\cdots w^{(N-1)}\right)\\ &= \left(A^{(1)} - \frac{1}{a}a^{(1)}\widetilde{a^{(1)}}\right)^{-1} = (A^{(1)})^{-1} + \frac{1}{a-x}(A^{(1)})^{-1}a^{(1)}\widetilde{a^{(1)}}(A^{(1)})^{-1}, \end{aligned} \tag{D.13}$$

where the Sherman-Morrison formula is used in the last step. Multiplying $\widetilde{a^{(1)}}$ from the left and $a^{(1)}$ from the right, we obtain

$$\widetilde{a^{(1)}}Ga^{(1)} = x + \frac{x^2}{a-x} = \frac{ax}{a-x}. \tag{D.14}$$

Using the definition of G and Eq. (C.10) for $a^{(1)}$ makes it possible to obtain

$$\widetilde{a^{(1)}}Ga^{(1)} = \widetilde{\zeta}A(1 - \zeta\widetilde{w})A^{-1}(1 - w\widetilde{\zeta})A\zeta = a^2\widetilde{w}A^{-1}w - a = \frac{a^2}{\alpha} - a \tag{D.15}$$

owing to Eqs. (C.6) and (C.7). Thus we obtain $x=a-\alpha$. From Eqs. (D.10) and (D.11), we have $\det A^{(1)}=(1/(a-x))(\det T)^2 \det A$, which is the first equality (D.6).

To prove the second equality (D.7), we start from Eq. (D.13), yielding the equation $G^{-1}=A^{(1)}-\frac{1}{a}a^{(1)}\widetilde{a^{(1)}}$. Inverting $A^{(1)}$ with use of the Sherman-Morrison formula leads to

$$(A^{(1)})^{-1} = (G^{-1} + \frac{1}{a}a^{(1)}\widetilde{a^{(1)}})^{-1} = G - \frac{1}{a+\widetilde{a^{(1)}}Ga^{(1)}}Ga^{(1)}\widetilde{a^{(1)}}G, \qquad (D.16)$$

where $a+\widetilde{a^{(1)}}Ga^{(1)}=a^2/\alpha$. The left side of Eq. (D.7) is thus expressed as

$$\left(\zeta^{(2)}\zeta^{(3)}\cdots\zeta^{(N-1)}\right)(A^{(1)})^{-1}\begin{pmatrix}\widetilde{\zeta^{(2)}}\\\widetilde{\zeta^{(3)}}\\\vdots\\\widetilde{\zeta^{(N-1)}}\end{pmatrix} = \left(\zeta^{(2)}\zeta^{(3)}\cdots\zeta^{(N-1)}\right)G\begin{pmatrix}\widetilde{\zeta^{(2)}}\\\widetilde{\zeta^{(3)}}\\\vdots\\\widetilde{\zeta^{(N-1)}}\end{pmatrix}$$

$$-\frac{\alpha}{a^2}\left(\zeta^{(2)}\zeta^{(3)}\cdots\zeta^{(N-1)}\right)Ga^{(1)}\widetilde{a^{(1)}}G\begin{pmatrix}\widetilde{\zeta^{(2)}}\\\widetilde{\zeta^{(3)}}\\\vdots\\\widetilde{\zeta^{(N-1)}}\end{pmatrix}. \qquad (D.17)$$

By using Eqs. (C.6) and (C.7) together with the definition of a and α, the first and second terms on the right side of Eq. (D.17) turn out to be

$$(1-\zeta\widetilde{w})A^{-1}(1-w\widetilde{\zeta}) = A^{-1} - \zeta\widetilde{w}A^{-1} - A^{-1}w\widetilde{\zeta} + \frac{1}{\alpha}\zeta\widetilde{\zeta},$$

$$-\frac{\alpha}{a^2}(1-\zeta\widetilde{w})A^{-1}(1-w\widetilde{\zeta})A\zeta\widetilde{\zeta}A(1-\zeta\widetilde{w})A^{-1}(1-w\widetilde{\zeta})$$

$$= -\frac{\alpha}{a^2}\left(A^{-1} - \zeta\widetilde{w}A^{-1} - A^{-1}w\widetilde{\zeta} + \frac{1}{\alpha}\zeta\widetilde{\zeta}\right)A\zeta\widetilde{\zeta}A\left(A^{-1} - \zeta\widetilde{w}A^{-1} - A^{-1}w\widetilde{\zeta} + \frac{1}{\alpha}\zeta\widetilde{\zeta}\right)$$

$$= -\alpha\left(\frac{1}{\alpha^2}\zeta\widetilde{\zeta} - \frac{1}{\alpha}A^{-1}w\widetilde{\zeta} - \frac{1}{\alpha}\zeta\widetilde{w}A^{-1} + A^{-1}w\widetilde{w}A^{-1}\right). \qquad (D.18)$$

Putting together these results completes the second equality (D.7).

D.3 Examples of nonlocal kernels

We here collect the matrix elements of typical nonlocal operators which appear in the RGM treatment for light nuclei. See Eq. (4.3) for the definition of the nonlocal operator.

(i) $V(\boldsymbol{r}',\boldsymbol{r}) = \exp\left(-\frac{1}{2}p'\boldsymbol{r}'^2 - \frac{1}{2}p\boldsymbol{r}^2 - q\boldsymbol{r}'\cdot\boldsymbol{r}\right)$

The nonlocal operator is nothing but $K(\boldsymbol{r}',\boldsymbol{r})$ of Eq. (C.1). Utilizing Eq. (C.16) we obtain

$$\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x}) \mid V_{\mathrm{NL}} \mid F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x})\rangle$$
$$= \langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x}) \mid [KF_{(L_1 L_2)LM}(u_1, u_2, A)](\boldsymbol{x})\rangle. \qquad (D.19)$$

As another method, it is possible to start from Eq. (4.4), yielding

$$\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x})|V_{\mathrm{NL}}|g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x})\rangle$$
$$= \left(\frac{(2\pi)^{N-2}c}{\det B}\right)^{\frac{3}{2}}\left(\frac{(2\pi)^2}{\det M}\right)^{\frac{3}{2}}\exp\left(\frac{1}{2}\widetilde{\boldsymbol{v}}J^{-1}\boldsymbol{v} + \frac{1}{2}\widetilde{\boldsymbol{Z}}M^{-1}\boldsymbol{Z}\right), \qquad (D.20)$$

where M is a 2×2 symmetric matrix defined by

$$M = \begin{pmatrix} \alpha+p & \beta+q \\ \beta+q & \alpha'+p' \end{pmatrix} \qquad (D.21)$$

with α, α', β being given in Eq. (4.6) and $\boldsymbol{Z}$ is a 2-dimensional vector whose elements are usual vectors defined by

$$\boldsymbol{Z}_1 = (\widetilde{\zeta} - \widetilde{\eta})\boldsymbol{s} - \widetilde{\eta}\boldsymbol{s}' = \sum_{i=1}^{4} \lambda_i \boldsymbol{e}_i f_1^{(i)}, \qquad \boldsymbol{Z}_2 = (\widetilde{\zeta} - \widetilde{\eta}')\boldsymbol{s}' - \widetilde{\eta}'\boldsymbol{s} = \sum_{i=1}^{4} \lambda_i \boldsymbol{e}_i f_2^{(i)}. \tag{D.22}$$

Here $f_1^{(i)}$ and $f_2^{(i)}$ are components of a 2-dimensional vector $f^{(i)}$:

$$f^{(i)} = \begin{pmatrix} \widetilde{\zeta}u_i - \widetilde{\eta}u_i \\ -\widetilde{\eta}'u_i \end{pmatrix} \text{ for } i = 1, 2, \qquad f^{(i)} = \begin{pmatrix} -\widetilde{\eta}u_i \\ \widetilde{\zeta}u_i - \widetilde{\eta}'u_i \end{pmatrix} \text{ for } i = 3, 4. \tag{D.23}$$

The desired matrix element is expressed in terms of the overlap matrix element (B.10) as

$$\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x}) \mid V_{\mathrm{NL}} \mid F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle$$
$$= \left(\frac{2\pi c}{\det M} \right)^{\frac{3}{2}} \langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x}) \mid F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle \Big|_{\rho_{ij} \to \chi_{ij}}, \tag{D.24}$$

where

$$\chi_{ij} = \widetilde{u}_i J^{-1} u_j + \widetilde{f^{(i)}} M^{-1} f^{(j)} = \bar{\rho}_{ij} + \widetilde{f^{(i)}} M^{-1} f^{(j)}. \tag{D.25}$$

As a straightforward application of the above formula, we consider a nonlocal operator $V(\boldsymbol{r}', \boldsymbol{r}) = \{\mathrm{erf}(\tau \mid \sigma\boldsymbol{r} + \sigma'\boldsymbol{r}' \mid)/\mid \sigma\boldsymbol{r} + \sigma'\boldsymbol{r}' \mid\} \exp\left(-p'\boldsymbol{r}'^2/2 - p\boldsymbol{r}^2/2 - q\boldsymbol{r}' \cdot \boldsymbol{r}\right)$ which often appears as the RGM kernel for the Coulomb potential. Using the relation (B.35), the operator is expressed as an integral of the nonlocal operator of type (i), so that its matrix element reduces to Eq. (D.19) with the replacement of p, p', q by

$$p \to p + 2\sigma^2\tau^2 t^2, \qquad p' \to p' + 2\sigma'^2\tau^2 t^2, \qquad q \to q + 2\sigma\sigma'\tau^2 t^2. \tag{D.26}$$

(ii) $V(\boldsymbol{r}', \boldsymbol{r}) = \left(\mathcal{Q}_{11}\boldsymbol{r}^2 + \mathcal{Q}_{22}\boldsymbol{r}'^2 + 2\mathcal{Q}_{12}\boldsymbol{r} \cdot \boldsymbol{r}' \right) \exp\left(-\frac{1}{2}p'\boldsymbol{r}'^2 - \frac{1}{2}p\boldsymbol{r}^2 - q\boldsymbol{r}' \cdot \boldsymbol{r}\right)$

Using Eq. (4.4) leads to the following expression

$$\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) | V_{\mathrm{NL}} | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle$$
$$= \left(3\mathrm{Tr} M^{-1}\mathcal{Q} + \widetilde{\boldsymbol{Z}} M^{-1}\mathcal{Q} M^{-1} \boldsymbol{Z} \right)$$
$$\times \left(\frac{(2\pi)^{N-2}c}{\det B} \right)^{\frac{3}{2}} \left(\frac{(2\pi)^2}{\det M} \right)^{\frac{3}{2}} \exp\left(\frac{1}{2}\widetilde{\boldsymbol{v}} J^{-1}\boldsymbol{v} + \frac{1}{2}\widetilde{\boldsymbol{Z}} M^{-1} \boldsymbol{Z} \right), \tag{D.27}$$

with

$$\mathcal{Q} = \begin{pmatrix} \mathcal{Q}_{11} & \mathcal{Q}_{12} \\ \mathcal{Q}_{12} & \mathcal{Q}_{22} \end{pmatrix}. \tag{D.28}$$

We can follow the steps of Eqs. (B.1), (B.11) and (B.14), and find that the desired matrix element is given by

$$\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x}) \mid V_{\mathrm{NL}} \mid F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle$$
$$= \left(\frac{2\pi c}{\det M} \right)^{\frac{3}{2}} \left(3\mathrm{Tr} M^{-1}\mathcal{Q} + 2 \sum_{j>i=1}^{4} h_{ij} \frac{\partial}{\partial \rho_{ij}} \right)$$
$$\times \langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x}) \mid F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle \Big|_{\rho_{ij} \to \chi_{ij}}, \tag{D.29}$$

where

$$h_{ij} = \widetilde{f^{(i)}} M^{-1} \mathcal{Q} M^{-1} f^{(j)}. \tag{D.30}$$

(iii) $V(\boldsymbol{r}', \boldsymbol{r}) = (-1)^{\ell}\sqrt{2\ell + 1}[\mathcal{Y}_{\ell}(\boldsymbol{r}')\mathcal{Y}_{\ell}(\boldsymbol{r})]_{00} \exp\left(-\frac{1}{2}p'\boldsymbol{r}'^2 - \frac{1}{2}p\boldsymbol{r}^2\right)$

As the last example, we consider a separable kernel which often appears in eliminating redundant states from the relative motion between the particles. Expressing $[\mathcal{Y}_{\ell}(\boldsymbol{r}')\mathcal{Y}_{\ell}(\boldsymbol{r})]_{00}$ as

$$[\mathcal{Y}_{\ell}(\boldsymbol{r}')\mathcal{Y}_{\ell}(\boldsymbol{r})]_{00} = \left(\frac{B_{\ell}}{\ell!} \right)^2 \int\int d\boldsymbol{e}' d\boldsymbol{e} [Y_{\ell}(\boldsymbol{e}')Y_{\ell}(\boldsymbol{e})]_{00} \frac{\partial^{2\ell}}{\partial\lambda^{\ell}\lambda'^{\ell}} \exp(\lambda\boldsymbol{e} \cdot \boldsymbol{r} + \lambda'\boldsymbol{e}' \cdot \boldsymbol{r}') \Big|_{\lambda = \lambda' = 0}, \tag{D.31}$$

we start from the matrix element between the generating functions

$$
\begin{aligned}
&\langle g(\lambda_3 \boldsymbol{e}_3 u_3 + \lambda_4 \boldsymbol{e}_4 u_4; A', \boldsymbol{x}) | V_{\mathrm{NL}} | g(\lambda_1 \boldsymbol{e}_1 u_1 + \lambda_2 \boldsymbol{e}_2 u_2; A, \boldsymbol{x}) \rangle \\
&= (-1)^\ell \sqrt{2\ell+1} \left(\frac{B_\ell}{\ell!} \right)^2 \int\int d\boldsymbol{e}' d\boldsymbol{e} [Y_\ell(\boldsymbol{e}')Y_\ell(\boldsymbol{e})]_{00} \frac{\partial^{2\ell}}{\partial\lambda^\ell\lambda'^\ell} \\
&\quad \times \left(\frac{(2\pi)^{N-2}c}{\det B} \right)^{\frac{3}{2}} \left(\frac{(2\pi)^2}{\det M_0} \right)^{\frac{3}{2}} \exp\left(\frac{1}{2}\tilde{\boldsymbol{v}}J^{-1}\boldsymbol{v} + \frac{1}{2}\widetilde{\boldsymbol{W}}M_0^{-1}\boldsymbol{W} \right)\Big|_{\lambda=\lambda'=0} \\
&\longrightarrow (-1)^\ell \sqrt{2\ell+1} \left(\frac{B_\ell}{\ell!} \right)^2 \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \left(\frac{2\pi c}{\det M_0} \right)^{\frac{3}{2}} \exp\left(\sum_{j>i=1}^4 \lambda_i\lambda_j\chi_{ij}\boldsymbol{e}_i\cdot\boldsymbol{e}_j \right) \\
&\quad \times \int\int d\boldsymbol{e}' d\boldsymbol{e} [Y_\ell(\boldsymbol{e}')Y_\ell(\boldsymbol{e})]_{00} \frac{\partial^{2\ell}}{\partial\lambda^\ell\lambda'^\ell} \\
&\quad \times \exp\left(\sum_{i=1}^4 \lambda\lambda_i\chi_1^{(i)}\boldsymbol{e}\cdot\boldsymbol{e}_i + \sum_{i=1}^4 \lambda'\lambda_i\chi_2^{(i)}\boldsymbol{e}'\cdot\boldsymbol{e}_i + (M_0^{-1})_{12}\lambda\lambda'\boldsymbol{e}\cdot\boldsymbol{e}' \right)\Big|_{\lambda=\lambda'=0}, \quad \text{(D.32)}
\end{aligned}
$$

where M_0 is obtained by putting $q=0$ in M of Eq. (D.21), and 2-component vectors $\chi^{(i)}$ and $\boldsymbol{W}$ are defined by

$$
\chi^{(i)} = M_0^{-1}f^{(i)} \quad (i=1,\ldots,4), \qquad \boldsymbol{W} = \begin{pmatrix} \boldsymbol{Z}_1 + \lambda\boldsymbol{e} \\ \boldsymbol{Z}_2 + \lambda'\boldsymbol{e}' \end{pmatrix}, \qquad \text{(D.33)}
$$

with $\boldsymbol{Z}_1$ and $\boldsymbol{Z}_2$ being defined in Eq. (D.22).

The desired matrix element is obtained from Eq. (3.2). To simplify the needed calculation, we introduce the following notations

$$
\begin{aligned}
&L_5 = L_6 = \ell, \qquad \boldsymbol{e}_5 = \boldsymbol{e}, \qquad \boldsymbol{e}_6 = \boldsymbol{e}', \qquad \lambda_5 = \lambda, \qquad \lambda_6 = \lambda', \\
&\chi_{i5} = \chi_1^{(i)}, \qquad \chi_{i6} = \chi_2^{(i)}, \qquad \chi_{56} = (M_0^{-1})_{12},
\end{aligned} \qquad \text{(D.34)}
$$

which make it possible to extend Eq. (3.2) to

$$
\begin{aligned}
&\langle F_{(L_3 L_4)L'M'}(u_3, u_4, A', \boldsymbol{x}) \mid V_{\mathrm{NL}} \mid F_{(L_1 L_2)LM}(u_1, u_2, A, \boldsymbol{x}) \rangle \\
&= (-1)^\ell \sqrt{2\ell+1} \left(\prod_{i=1}^6 \frac{B_{L_i}}{L_i!} \right) \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \left(\frac{2\pi c}{\det M_0} \right)^{\frac{3}{2}} \\
&\quad \times \int\cdots\int \prod_{i=1}^6 d\boldsymbol{e}_i ([Y_{L_3}(\boldsymbol{e}_3)Y_{L_4}(\boldsymbol{e}_4)]_{L'M'})^* [Y_{L_1}(\boldsymbol{e}_1)Y_{L_2}(\boldsymbol{e}_2)]_{LM} [Y_{L_5}(\boldsymbol{e}_5)Y_{L_6}(\boldsymbol{e}_6)]_{00} \\
&\quad \times \left(\prod_{i=1}^6 \frac{\partial^{L_i}}{\partial\lambda_i{}^{L_i}} \right) \exp\left(\sum_{j>i=1}^6 \lambda_i\lambda_j\chi_{ij}\boldsymbol{e}_i\cdot\boldsymbol{e}_j \right)\Big|_{\lambda_i=0}. \qquad \text{(D.35)}
\end{aligned}
$$

The above operation can be performed similarly to the overlap case, yielding a formula

$$\langle F_{(L_3 L_4) L' M'}(u_3, u_4, A', \boldsymbol{x}) \mid V_{\mathrm{NL}} \mid F_{(L_1 L_2) L M}(u_1, u_2, A, \boldsymbol{x}) \rangle$$

$$= \delta_{LL'} \delta_{MM'} (-1)^{L_1 + L_2 + \ell} \sqrt{\frac{2\ell + 1}{2L + 1}} \left(\prod_{i=1}^{6} B_{L_i} \right) \left(\frac{(2\pi)^{N-1}}{\det B} \right)^{\frac{3}{2}} \left(\frac{2\pi c}{\det M_0} \right)^{\frac{3}{2}}$$

$$\times \sum_{p_{ij}} \left(\prod_{j>i=1}^{6} \frac{(-1)^{p_{ij}} \sqrt{2p_{ij}+1}}{B_{p_{ij}}} (\chi_{ij})^{p_{ij}} \right)$$

$$\times \sqrt{\frac{(2L+1)(2L_5+1)}{(2p_{56}+1)(2L_5-2p_{56}+1)}} \left[\begin{array}{ccc} p_{12} & p_{12} & 0 \\ L_1-p_{12} & L_2-p_{12} & L \\ L_1 & L_2 & L \end{array} \right] \left[\begin{array}{ccc} p_{34} & p_{34} & 0 \\ L_3-p_{34} & L_4-p_{34} & L \\ L_3 & L_4 & L \end{array} \right]$$

$$\times C(p_{12} \ L_1-p_{12}; L_1) \, C(p_{13}+p_{14} \ p_{15}+p_{16}; L_1-p_{12})$$

$$\times C(p_{12} \ L_2-p_{12}; L_2) \, C(p_{23}+p_{24} \ p_{25}+p_{26}; L_2-p_{12})$$

$$\times C(p_{34} \ L_3-p_{34}; L_3) \, C(p_{13}+p_{23} \ p_{35}+p_{36}; L_3-p_{34})$$

$$\times C(p_{34} \ L_4-p_{34}; L_4) \, C(p_{14}+p_{24} \ p_{45}+p_{46}; L_4-p_{34})$$

$$\times C(p_{56} \ L_5-p_{56}; L_5) \, C(p_{15}+p_{25} \ p_{35}+p_{45}; L_5-p_{56})$$

$$\times C(p_{56} \ L_6-p_{56}; L_6) \, C(p_{16}+p_{26} \ p_{36}+p_{46}; L_6-p_{56})$$

$$\times \sum_{\lambda \lambda'} \frac{1}{\sqrt{(2\lambda+1)(2\lambda'+1)^3}} X(p_{13}p_{14}p_{23}p_{24}; \lambda) X(p_{15}p_{16}p_{25}p_{26}; \lambda') X(p_{35}p_{36}p_{45}p_{46}; \lambda')$$

$$\times \left[\begin{array}{ccc} p_{13}+p_{14} & p_{23}+p_{24} & \lambda \\ p_{15}+p_{16} & p_{25}+p_{26} & \lambda' \\ L_1-p_{12} & L_2-p_{12} & L \end{array} \right] \left[\begin{array}{ccc} p_{13}+p_{23} & p_{14}+p_{24} & \lambda \\ p_{35}+p_{36} & p_{45}+p_{46} & \lambda' \\ L_3-p_{34} & L_4-p_{34} & L \end{array} \right]$$

$$\times \left[\begin{array}{ccc} p_{15}+p_{25} & p_{16}+p_{26} & \lambda' \\ p_{35}+p_{45} & p_{36}+p_{46} & \lambda' \\ L_5-p_{56} & L_6-p_{56} & 0 \end{array} \right], \tag{D.36}$$

where non-negative integers p_{ij} satisfy the following equations

$$p_{12} + p_{13} + p_{14} + p_{15} + p_{16} = L_1, \qquad p_{12} + p_{23} + p_{24} + p_{25} + p_{26} = L_2,$$
$$p_{13} + p_{23} + p_{34} + p_{35} + p_{36} = L_3, \qquad p_{14} + p_{24} + p_{34} + p_{45} + p_{46} = L_4,$$
$$p_{15} + p_{25} + p_{35} + p_{45} + p_{56} = L_5, \qquad p_{16} + p_{26} + p_{36} + p_{46} + p_{56} = L_6. \tag{D.37}$$

There are 15 p_{ij}, which satisfy 6 conditions. Thus we have in general 9 independent p_{ij} in contrast to 2 in the overlap case. In the case of natural parity states, however, because of $L_2 = L_4 = 0$ only two of p_{ij}, e.g., p_{13} and p_{15} are independent.

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